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Materials Sciences Programs

Fiscal Year 1997

U.S. Department of Energy
Office of Science
Office of Basic Energy Sciences
Division of Materials Sciences
Germantown Building
19901 Germantown Road
Germantown, MD 20874-1290

FOREWORD

The Division of Materials Sciences is located within the Department of Energy (DOE) in the Office of Basic Energy Sciences which is under the Office of Science. The Director of the Office of Science is appointed by the President and confirmed by the Senate. The Director of the Office of Science is responsible for oversight of, and providing advice to, the Secretary of Energy on the Department's research portfolio and on the management of all of the Laboratories that it owns, except for those that are designated as having a primary role in nuclear weaponry.

The Division of Materials Sciences is responsible for basic research and research facilities in materials science topics important to the mission of the Department. The programmatic divisions under the Office of Basic Energy Sciences are Chemical Sciences, Engineering and Geosciences, and Energy Biosciences; information for them is contained on page 190. Materials Science is an enabling technology. The performance parameters, economics, environmental acceptability and safety of all energy generation, conversion, transmission and conservation technologies are limited by the properties and behavior of materials. The Materials Sciences programs develop scientific understanding of the synergistic relationship among synthesis, processing, structure, properties, behavior, performance and other characteristics of materials. Emphasis is placed on the development of the capability to discover technologically, economically, and environmentally desirable new materials and processes, and the instruments and national user facilities necessary for achieving such progress. Materials Sciences sub-fields include: physical metallurgy, ceramics, polymers, solid state and condensed matter physics, materials chemistry, surface science and related disciplines where the emphasis is on the science of materials.

This report includes program descriptions for 517 research programs including 255 at 14 DOE National Laboratories, 262 research grants (233 of which are at universities), and 29 Small Business Innovation Research Grants. Five cross-cutting indices located at the rear of this book identify all 517 programs according to principal investigator(s), materials, techniques, phenomena, and environment. Other contents include identification of our Staff structure and expertise on pages ii-iii; a bibliographical listing of 50 scientific workshop, topical, descriptive, Research Assistance Task Force and research facilities reports on select topics that identify materials science research needs and opportunities on pages iv - viii; a descriptive introduction on page ix; a descriptive summary of the DOE Center of Excellence for the Synthesis and Processing of Advanced Materials is on pages 121-126; and a descriptive summary and access information on 14 national research user facilities including synchrotron light sources, neutron beam sources, electron beam microcharacterization instruments, materials preparation, surface modification, and combustion research is on pages 128-163.

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

OFFICE OF BASIC ENERGY SCIENCES
DIVISION OF MATERIALS SCIENCES

IRAN L. THOMAS
DIRECTOR

CHRISTIE L. ASHTON - SECRETARY
(301) 903-3427

METAL AND CERAMICS SCIENCES TEAM

ROBERT J. GOTTSCHALL
LEADER

ALAN L. DRAGOO
WENDY R. CIESLAK*
TIMOTHY J. FITZSIMMONS
CRAIG S. HARTLEY*
YOK CHEN
HELEN M. KERCH

MARY STOWERS - SECRETARY
(301) 903-3428

CONDENSED MATTER PHYSICS AND MATERIALS CHEMISTRY TEAM

WILLIAM T. OOSTERHUIS
LEADER

RICHARD D. KELLEY
JERRY J. SMITH
JEFF HOY
MATESH VARMA
DON LIEBENBERG*
MANFRED LEISER
DONNA PROKOP

MELANIE BECKER - SECRETARY
(301) 903-3426

* ON DETAIL
FAX NUMBER: (301) 903-9513

EMAIL ADDRESS: FIRSTNAME.LASTNAME@OER.DOE.GOV

HTTP://WWW.ER.DOE.GOV/PRODUCTION/BES/DMS

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

Metals and Ceramic Sciences Team, ER-131

Name	Program Area
Robert J. Gottschall	Electron Beam Microcharacterization Facilities
Alan L. Dragoo	Ceramics
Yok Chen	Physical Behavior, Irradiation Effects
Timothy J. Fitzsimmons	Ceramics, High Temperature Superconductors, High Temperature Materials
Helen M. Kerch	Microstructure, Processing
Wendy R. Cieslak	Corrosion, Electrochemistry, Tribology, Adhesion, Modeling and Simulation
Craig S. Hartley	Mechanical Engineering, Metallurgical Research, Materials Sciences, Residual Stress, Defects, Mechanical Behavior of Materials

Condensed Matter Physics and Materials Chemistry Team, ER-132

Name	Program Area
William T. Oosterhuis	Neutron and X-ray Facilities
Richard D. Kelley	Materials Chemistry, Polymers, Surface Science
Jerry J. Smith	Solid State Physics, Surface Science
Manfred Leiser	Solid State Theory
Jeff Hoy	Scientific Facility Construction Management, Nuclear Engineering, Magnetic Plasma Confinement Systems, Ocean Engineering
Donna J. Prokop	EPSCoR Program
Matesh Varma	Solid State Physics, Atomic Physics, Radiation Sciences, Biophysics, Surface Physics, Instrumentation, Environmental Management Science, Medical Applications, Computational Structural Biology

E-Mail Address:

firstname.lastname@oer.doe.gov

Fax Number:

301/903-9513

Regular Mail and Federal Express:

Division of Materials Sciences, ER-__
Office of Basic Energy Sciences
U.S. Department of Energy
19901 Germantown Road
Germantown, Maryland 20874-1290

WORKSHOP AND REPORT 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 15 years. The contributions to them come from scientists drawn from universities, national laboratories, and industry, and represent a diverse mixture as well as a balance of sub-disciplines within materials science. It is our intention to make the proceedings of these activities publicly available through publication in open literature scientific journals, bulletins, or other archival forms. Many of these publications identify the authors perceptions of emerging or existing generic materials science research needs and opportunities. Their primary purpose is to stimulate creative thinking and new ideas by scientists within their respective topical fields. None of these 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 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.

"Radiation Effects in Crystalline Ceramics for the Immobilization of High-Level Nuclear Waste and Plutonium," W. J. Weber, R. C. Ewing, C. R. A. Catlow, T. Diaaz de la Rubia, L. W. Hobbs, C. Kinoshita, H. J. Matzke, A. T. Motta, M. A. Nastasi, E. H. K. Salje, E. R. Vance, and S. J. Zinkle, J. Mater. Res., 13, 6 June 1988.

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"Ordered Intermetallic Alloys: An Assessment," C. T. Liu, J. Stringer, J. N. Mundy, L. L. Horton, and P. Angelini. Intermetallics 5 (1997) 579-596.

"Current Issues in Recrystallization: A Review," R. D. Doherty, D. A. Hughes, F. J. Humphreys, J. J. Jonas, D. Juul Jensen, M. E. Kassner, W. E. King, T. R. McNelley, H. J. McQueen, A. D. Rollett, Journal of Materials Science and Engineering, Volume 238/2 of Mat. Sci. Eng. A pages 219-274.

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"Applications of Positron Spectroscopy to Materials Science," L.D.Hulett,Jr, R. Gonzalez, B.L.Brown, A.L.Denison, R.H.Howell, Y.C.Jean, P.L.Jones, W.J.Kossler, K.G.Lynn, A.P.Mills Jr., S.Okada, D.M.Schrader, L.C.Smedskjaer, A.H.Weiss, R.N.West and Y.Chen, Advanced Materials Research, Vol 3, pp 1 - 67 (1994).

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"Grain Boundary and Interface Phenomena in the High-Temperature Plasticity of Solids," M. E. Kassner and T. G. Langdon, editors, Materials Science and Engineering, 166, pp 1-246, 1993 (23 paper dedicated issue).

"Radiation Effects in Glasses Used for the Immobilization of High-Level Waste and Plutonium Disposition," W. J. Weber, R. C. Ewing, C. A. Angell, G. W. Arnold, A. N. Cormack, J. M. Delaye, D. L. Griscom, L. W. Hobbs, A. Navrotsky, D. L. Price, A. M. Stoneham, and M. C. Weinberg, Journal of Materials Research, Mater. Res. Vol. 12, No. 8 (1997) in press.

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"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.

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"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.

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

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Description of Research Facilities, Plans, and Associated Programs

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"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 eight 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, Section D describes the Center of Excellence for the Synthesis and Processing of Advanced Materials and E has information on major user facilities. F describes other user facilities, G as a summary of funding levels and H has indices characterizing research projects.

The FY 1997 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 Metals and Ceramic Sciences (01), Condensed Matter Physics (02), Materials Chemistry (03), or Facility Operations (04). The budget numbers carry the following titles:

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

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

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

04-1 - Facility Operation

For more detailed information call (301) 903-3428 for the Metals and Ceramic Sciences topics; (301) 903-3426 for the Condensed Matter Physics and Materials Chemistry topics.

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

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

Preparation of this FY 1997 summary report was coordinated by Iran L. Thomas. The effort required time by every member of the Division. Much of the work was done by Christie Ashton.

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SECTION A

Laboratories

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

AMES LABORATORY

Iowa State University
Ames, IA 50011

D. Hoffman - (515) 294-9649
Fax: (515) 294-4456

Metallurgy and Ceramics - 01 -

I. Anderson - (515) 294-4446
Fax: (515) 294-4456

1. CONTROLLED MICROSTRUCTURES

I. E. Anderson
(515) 294-4446 01-1 $199,100

Studies to improve the performance of materials by achieving enhanced control of composition and microstructure during processing that involves diffusion and deformation with emphasis on powder-based materials. Perform hot isostatic pressing (HIP) experiments on high pressure gas atomized (HPGA) quasicrystalline Al-Cu-Fe powder to develop fabrication process for monolithic and composite forms of this novel material. Investigate consolidation by HIP and vacuum sintering of unique Al powders that contain high supersaturations of reactive gas resulting from gas atomization reaction synthesis (GARS) processing in the HPGA to form refractory dispersoid reinforced composites. Study consolidation of intermetallic powders to produce bulk shapes with technologically useful levels of toughness and strength. This program participates in the focus project on Tailored Microstructures in Hard Magnets of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

2. SOLIDIFICATION MICROSTRUCTURES

R. K. Trivedi, L. S. Chumbley, D. C. Jiles, R. W. McCallum
(515) 294-5869 01-1 $653,900

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. Dissociation/recombination phenomena in intermetallic compounds exposed to inductively coupled plasma. 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. This program participates in the focus project on Tailored Microstructures in Hard Magnets of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

3. MARTENSITIC PHASE TRANSFORMATIONS

B. N. Harmon, K. M. Ho, J. R. Morris
(515) 294-7712 01-2 $129,000

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. Modeling pseudoelastic and thermoelastic behaviors of shape-memory alloys. Investigation of twin formation and its affects on ductility in hcp metals. Application of molecular dynamics using realistic interatomic potentials. Study of prototypical systems: Na, NiTi, NiAl, Ba, Zr, TiPd, etc. Development and use of the algorithm for complex defect structure optimization.

4. MECHANICAL BEHAVIOR OF MATERIALS

O. Unal, B. Biner, J. Kameda
(515) 294-4892 01-2 $426,000

Studies of the effects of environment and stress on the mechanical properties and corrosion of ultra-high temperature materials. High-temperature-induced intergranular cracking in Ni base alloys. Description of three dimensional arrays of defects and relationship of arrangement to ductility and creep. Correlation between defect structure and nondestructive measurement. Effects of post-irradiation annealing on mechanical properties.

5. RARE EARTH AND RELATED MATERIALS

K. A. Gschneidner, Jr., V. Pecharsky
(515) 294-7931 01-3 $295,000

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

6. ADVANCED MATERIALS AND PROCESSES
I. E. Anderson, M. Akinc, L. L. Jones,
T. A. Lograsso, D. J. Sordelet,
R. K. Trivedi
(515) 294-4446 01-5 $930,900

Development of advanced processes for preparing specialty metals. Development of new melting procedures for preparing metal matrix composites. New thermite reduction process for preparing rare earth-iron alloys and for producing permanent magnet and magnetostrictive alloys. Processing of stoichiometric and non-stoichiometric materials by an inductively coupled plasma. Electrotransport and zone melting for maximum purification of rare earth and refractory metals. Processing of single crystals of congruent melting and peritectic materials by levitation zone melting, free-standing vertical zone melting, Bridgman, Czochralski and strain-anneal recrystallization. High pressure gas atomization for production of fine powders of metals and mixed metal oxides. Specialized coatings by plasma-arc spraying. Ceramic-ceramic bonding. Research above supports directly the Materials Preparation Center described in the Facilities Section. This program participates in the focus project on Materials Joining of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

7. NDE MEASUREMENT TECHNIQUES
O. Buck, D. C. Jiles, C. H. Schilling,
R. B. Thompson
(515) 294-9998 01-5 $398,600

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. X-ray microfocus techniques for high resolution studies of green microstructure and defects. Effects of fatigue damage, stress and microstructure on magnetic properties, particularly Bloch wall motion. This program participates in the focus projects on Metal Forming and Materials Joining of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

8. MAGNETOCALORIC MATERIALS AND THEIR PREPARATION
K. A. Gschneidner, Jr., I. E. Anderson,
V. K. Percharsky
(515) 294-7931 01-5 $174,000

Properties of rare earth-based alloys with magnetocaloric effect (MCE). Measure heat capacity as a function of temperature. Enhance and tailor the MCE in known and new rare earth-based metallic materials. Investigate scientific issues in processing technologies relevant to maximizing heat transfer capabilities of these materials. Current approach is to evaluate experimental quantities of atomized MCE particulates.

9. SCIENTIFIC AND TECHNOLOGICAL INFORMATION EXCHANGE
L. L. Jones, T. A. Lograsso, S. Mitra
(515) 294-5236 01-5 $163,000

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

10. MATERIALS PREPARATION CENTER
L. L. Jones, D. P. Baldwin,
T. A. Lograsso
(515) 294-5236 01-5 $232,000

It has and continuously develops unique capabilities for preparation, purification, fabrication, and characterization of a wide variety of metals and materials by processes that have been discovered or utilized by investigators at the Ames Laboratory during the course of their basic research. The Center provides laboratory research quantities of research grade materials not available in specific forms or purities from commercial suppliers on a full cost recovery basis. Expertise in very pure rare earths, alkaline earths, refractory metals, and some actinide metals. Forms of materials available include single crystals, bi-crystals, cast ingots, atomized powders, wires, rods, and sheets. Assures research community access to materials of the highest possible quality for their research programs. Center also has an Analytical Section for chemical and spectrographic analysis. Upgrad of existing processing equipment and capabilities through support from the Scientific Facilities Initiative (see Facilities section in this booklet).

11. FUNDAMENTALS OF PROCESSING OF BULK HIGH-T_C SUPERCONDUCTORS
R. W. McCallum, J. R. Clem,
D. K. Finnemore, D. C. Johnson,
M. J. Kramer
(515) 294-4736 01-5 $454,500

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. Thermal and quantum fluctuations of vortices. This program participates in the focus project on Materials Joining of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

12. ENVIRONMENTALLY-BENIGN GELCASTING OF CERAMICS
C. H. Schilling, L. Ukrainczyk
(515) 294-9465 01-5 $134,000

Interface chemistry involved in regulating plasticity during gelcasting of ceramics. Utilize ultra fine alumina as model ceramic particulate material. Investigate fundamental basis for use of modified starches as plasticizers. Measure electrophoretic mobility of particulate/additive aqueous suspensions. Utilize thermal analysis and diffuse reflectance infrared Fourier transform spectroscopy to reveal complexation mechanisms of powder surfaces in suspensions. Characterize effects by evaluation of rheology, green-body mechanical properties, and sintering behavior.

Solid State Physics - 02 -

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

13. NEUTRON SCATTERING
C. Stassis, A. R. Goldman, D. Vaknin,
J. Zarestky
(515) 294-4224 02-1 $410,000

Study of the magnetic properties of high temperature superconductors and related compounds by polarized and unpolarized neutron scattering techniques (La_2CuO_4, $LaNiO_4$, $La_{2-x}Sr_xCuO_4$, $La_{2-x}Sr_xNiO_4$), Sr_2Cl_2, $Ca_2Cl_2CuO_2$, and $BaCuO_2$. Study of magnetism and superconductivity in the $RENi_2C_2B$ systems. Experimental investigation of the lattice dynamics of metals and alloys undergoing martensitic transformations (bcc La, Cu-Al-Be, Cu-Al-Ni, Cu-Zn-Al); study of the Verwey transition in magnetite. Electronic structure and phonon spectra of mixed valence compounds ($CePd_3$, $_y$-Ce). Lattice dynamics of quasicrystals. Study of organic films on aqueous and solid surfaces by neutron and X-ray diffraction techniques.

14. NEW MATERIALS AND PHASES
F. Borsa, D. C. Johnston, L. L. Miller,
C. A. Swenson
(515) 294-5435 02-2 $450,000

Synthesis and characterization of new high-T_c superconductors, related oxides, and strongly correlated electron systems. Study of the physical properties of these new materials, such as phase equilibria and high and low temperature behavior. Properties of new phases including magnetic susceptibility, transport properties, heat capacity, crystallographic phase transformations, coexistence and/or competition of superconductivity and magnetic order. Modeling and analysis of the data using appropriate theories. High pressure equations of state of new materials, elementary solids (ternary compounds and alloys, and alkaline earth metals), low temperature expansivity and heat capacity of materials containing hydrogen. Applications of NMR to high-T_c superconductors, and strongly correlated electronic systems. Low dimensional magnetic systems (including magnetic molecular clusters), and phase transitions. NMR studies of ionic motion in superionic conductors and of hydrogen motion in quasicrystals.

15. MAGNETIC MATERIALS
P. Canfield, A. I. Goldman,
K. A. Gschneidner, B. N. Harmon,
D. W. Lynch, C. Stassis
(515) 294-7712 02-2 $475,000

Synthesis and detailed characterization of new magnetic materials. Study of magnetic structures in exotic materials using magnetic X-ray diffraction and neutron scattering. Investigation of the correlation, spin-orbit, and exchange interactions leading to novel or large magneto-optical properties. Kerr angle spectroscopy development and use of circular magnetic X-ray dichroism as a new tool for studying local magnetic properties. Theoretical modeling, first principles calculations, and predictions in close collaboration with the experimental effort. Specific families of materials include single crystalline: R=RE.

16. SUPERCONDUCTIVITY
D. K. Finnemore, J. E. Ostenson
(515) 294-3455 02-2 $190,000

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, fundamental studies of vortex motion; 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 superconducting composites with very strong pinning suitable for large scale magnets in the 8 to 16 Tesla range, practical studies to improve wire fabrication techniques.

17. X-RAY DIFFRACTION PHYSICS
A. I. Goldman
(515) 294-3585 02-2 $350,000

X-ray measurements on Icosahedral Phase alloys. Magnetic structures and phase transitions, and solids at high pressure. Magnetic X-ray scattering and spectroscopy. Study of magnetism and superconductivity in the $RENi_2C_2B$ systems.

18. PHOTONIC BAND GAP MATERIALS
K.-M. Ho, R. Biswas, K. Constant,
W. Leung, C. M. Soukoulis, G. Tuttle
(515) 294-1960 02-2 $520,000

Fabrication and design of materials with periodically varying dielectric constants. Design of photonic crystals with metallic elements and intentional 'defects'. Enhancement and suppression of radiative transition rates. Antennas. Resonant Filters and Detectors.

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

Electron photoemission, and optical properties (transmission, reflection, ellipsometry, Kerr spectroscopy) of solids in the visible, vacuum ultraviolet and soft X-ray region using synchrotron radiation. Ce and Ce-compounds Ce_2Sb, CeSb, $CeSb_2$, copper-oxide-based superconductors, quasicrystals. Epitaxial growth on metal and semiconductor surfaces, surface diffusion, ultrathin film morphology, LEED (Low Energy Electron Diffraction), RHEED (Reflection, High Energy Electron Diffraction), STM (Scanning Tunneling Microscopy) are used for structural characterization and growth measurements (Ag/Ag(lll), Ag/Si(lll), O/Si(iii)).

20. SEMICONDUCTOR PHYSICS
J. Shinar
(515) 294-8706 02-2 $160,000

(i) Fabrication and studies of pi-conjugated thin films and devices by UV-Vis-NIR absorption, photoluminescence, electroluminescence, transport, and optically and electrically detected magnetic resonance (ODMR and EDMR, respectively). (ii) Fabrication of hydrogenated amorphous Si- and C-based thin films, and studies of their hydrogen dynamics using secondary ion mass spectrometry (SIMS), IR, and small angle X-ray scattering (SAXS). (iii) Studies of porous Si films and devices using luminescence, ODMR, and EDMR spectroscopies.

21. SUPERCONDUCTIVITY THEORY
J. R. Clem, V. Kogan
(515) 294-4223 02-3 $260,000

Theoretical investigations of the electrodynamic behavior of superconductors, especially while carrying electrical current in magnetic fields. Research focuses on type-II superconductors with an emphasis on the high-temperature copper-oxide superconductors. Topics under study include vortex structure in layered materials, transitions between different vortex-lattice structures, fluctuations, vortex dynamics, 2D pancake vortices, magnetic-flux penetration into thin films, weak-link effects, surface impedance, ac losses, surface barriers, and flux-line cutting.

22. ELECTRONIC AND MAGNETIC PROPERTIES
B. N. Harmon, K.-M. Ho, M. Luban,
C. M. Soukoulis
(515) 294-7712 02-3 $330,000

Theoretical studies of structural and lattice dynamical properties of cluster and bulk materials using first principles total energy calculations. Magnetic properties of new R=RE superconductors. Anharmonic interactions, lattice instabilities, phase transformations, electron-phonon interaction, and superconductivity. Equations of state (pressure and temperature). Electron and light localization in quasi-periodic, disordered, and nonlinear 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. Wave propagation in random media. Theoretical modeling of quantum dot nanostructures and Bloch oscillations. Buckyballs and other carbon structures. Spin relaxation in mesoscopic magnets.

23. SPIN DYNAMICS
B. N. Harmon, V. Antropov
(515) 294-0698 02-3 $250,000

A joint computational materials sciences effort between AL and ORNL to develop first principles electronic structure techniques for the study of large scale magnetic properties, including temperature dependent dynamics, giant magneto resistance, multilayers, and changes in spin coupling strengths caused by defects. Treatment of unit cells containing hundreds or thousands of atoms requires modern supercomputing facilities.

24. OPTICAL AND SURFACE PHYSICS THEORY
K.-M. Ho, G. D. Lee
(515) 294-1960 02-3 $165,000

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

25. MUCAT SECTOR AT THE ADVANCED PHOTON SOURCE
A. I. Goldman, D. W. Lynch,
D. Robinson
(515) 294-8700 02-5 $1,000,000

Design and construction of the undulator beamline at the Advanced Photon Source (APS). Design of optical elements of modifying the polarization of the undulator radiation and polarization analysis of the scattered beam. Testing and certification of components constructed for use at the APS. Experiments in magnetic scattering, surface sciences, and diffraction using undulator radiation.

Materials Chemistry - 03 -

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

26. SYNTHESIS AND CHEMICAL STRUCTURE
J. D. Corbett, J. W. Anderegg,
H. F. Franzen, R. A. Jacobson,
R. E. McCarley
(515) 294-3086 03-1 $642,000

Synthesis, structure and bonding in polar intermetallic systems. Interstitial derivatives of intermetallic phases - the systematic variation of electronic, conduction, and magnetic properties and corrosion resistance. Influence of common impurities (O, N, H) on stability of intermetallic compounds. Homoatomic clusters of main-group metals in condensed phases; electronic regularities. Zintl phases, criteria and property relationships. Synthesis, bonding, structure and properties of new reduced ternary oxide and chalcogenide 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, especially metastable crystalline and amorphous phases. Structure and properties of new higher valent transition metal nitrides. Electronic band structure calculations. Study of refractory metal-rich binary and ternary sulfides and oxides by both experimental and theoretical techniques to understand the relationships among crystal structure, chemical bonding, and electronic structure as they affect high temperature stability, phase equilibria, and order-disorder transitions. Development of diffraction techniques for single crystal and non-single crystal specimens, techniques for pulsed-neutron and synchrotron radiation facilities, and use of Patterson superposition methods. Experimental methods: X-ray and electron diffraction, X-ray and UV photoelectron spectroscopy, resistivity and magnetic susceptibility measurements, computer automated mass-loss-mass-spectrometry for high-temperature vaporation reactions.

27. POLYMER AND ENGINEERING CHEMISTRY
T. J. Barton, M. Akinc,
S. Ijadi-Maghsoodi, V. V. Sheares
(515) 294-2770 03-2 $433,000

Synthesis of highly-strained, unsaturated, organometallic rings for ring-opening polymerizations. Study of controlled thermal decomposition of preceramic polymers. Development of thermal and photo-chemical routes to transient compounds containing silicon 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 processing of novel intermetallics for high temperature structural applications. Oxidation behavior of ternary silicides. Study of thermomechanical properties of novel ternary silicides. Study of step growth polymers. Synthesis of a soluble poly(p-phenylene) derivative.

28. HIGH TEMPERATURE AND SURFACE CHEMISTRY
P. A. Thiel, C. J. Jenks, D. C. Johnson
(515) 294-8985 03-3 $334,000

Surface phenomena in quasicrystals. Mechanisms of oxidation of metals and alloys, and properties of oxide overlayers (composition, stability, structure). Chemistry of electrode reactions, including electrocatalysis, electrochemical incineration, and corrosion reactions. Characterization of electrocatalytic materials by modulated hydrodynamic voltammetry. Reactivity of oxidized and doped electrode surfaces, including characterization of oxygen mobility and defect density at such electrodes. Equilibrium and dynamic properties of adsorbed films. Techniques used include low energy electron diffraction, Auger electron spectroscopy, electron energy loss spectroscopy, temperature programmed desorption, electron-stimulated desorption, X-ray photoelectron spectroscopy, scanning tunneling microscopy, ring-disk and modulated hydrodynamic voltammetry.

29. SURFACE AND INTERFACE PROPERTIES OF QUASICRYSTALS
P. A. Thiel, J. W. Anderegg, M. F. Besser, T. Bloomer, D. W. Delaney, A. I. Goldman, C. J. Jenks, M. J. Kramer, T. A. Lograsso, D. J. Sordelet, M. A. Van Hove
(515) 294-8985 03-3 $486,000

Studies of surface and interface properties of quasicrystals. Preparation of large, single-phase, well-defined samples of icosahedral AlPdMn and AlCuFe. Phase transformations within AlCuFe powders. Friction and wear at coatings and single-grain samples. Surface structure determination using low-energy electron diffraction. Surface oxidation. Oxidation state of grain boundaries in plasma sprayed samples and subsequent heat-treated samples. Microstructure of plasma sprayed coatings with and without additions.

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, IL 60439

F. Y. Fradin - (630) 252-3504
Fax: (630) 252-6720

Metallurgy and Ceramics - 01 -

B. D. Dunlap - (630) 252-4925
Fax: (630) 252-4798

30. ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH
M. A. Kirk, C. W. Allen
(630) 252-4998 01-1 $1,652,000

Development and use of high-voltage, high-spatial resolution and advanced analytical microscopy for materials research. Operation and development of the Center's HVEM-Tandem Facility with in-situ high voltage and intermediate voltage electron microscope capability for direct observation of ion-solid interactions. The HVEM and IVEM are currently being utilized for research programs in irradiation effects in advanced materials and mechanical properties. Specimen holders are available for heating (to 1100 K), cooling (to 10 K), and straining of specimens in-situ. Ion-beam interfaces with 650 kV ion implanter and 2 MV tandem accelerator available for in-situ implantations and irradiations into the HVEM or IVEM. More than 50 percent of HVEM usage is by non-ANL scientists for research proposals approved by the Steering Committee for the Center. A medium-voltage, ultra-high vacuum, field-emission gun, Analytical Electron Microscope has recently been installed. Its design is directed toward the attainment of the highest microanalytical resolution and sensitivity Fundamental studies of electron-solid interactions and microcharacterization of materials, using TEM, STEM, HREM, CBED, XEDS, and EELS are conducted on conventional transmission electron microscopes (JEOL 4000 EXII, JEOL 100CXII, Phillips EM420, and Phillips CM30).

31. INTERFACES IN ADVANCED CERAMICS
D. Wolf, D. Auciello, J. A. Eastman,
K. L. Merkle, S. R. Phillpot
(630) 252-5205 01-3 $1,572,000

Experimental synthesis and characterization methods are combined with atomistic computer simulation techniques to address fundamental issues relevant to the synthesis, characterization and elucidation of interfacially controlled properties of oxide and nitride ceramic thin films. The program focuses on four scientific themes:
(a) Microstructure and composition control during synthesis and processing of oxide and nitride thin films, for example, in-situ x-ray studies at the Advanced Photon Source (APS); (b) Characterization of interfacial strains, including the identification of modes of strain relaxation during in-situ growth and/or post-growth environmental re-equilibration at the APS and the effects of such strains on the phase diagram; (c) Determination of the atomic structure and chemistry of interfaces in these films, including the structure and composition of amorphous intergranular films in covalently bonded ceramics, the effects of severe microstructural constraints (e.g., associated with a small film thickness or a nanometer-scale grain size), and the mechanism(s) of interfacial off-stoichiometry accommodation as a function of film microstructure and thickness; (d) Correlation of "structure" and properties: film adhesion and corrosion-and-wear resistance as a function of interfacial strains, film microstructure, thickness and composition, and atomic structure and composition of the interface. This program participates in the focus projects on Materials Joining and High Efficiency Photovoltaics of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

32. IRRADIATION AND KINETIC EFFECTS
L. E. Rehn, D. E. Alexander,
R. C. Birtcher, S. K. Chan, N. Q. Lam,
P. R. Okamoto, N. J. Zaluzec
(630) 252-5021 01-4 $1,499,000

Investigations of mechanisms leading to the formation of defect aggregates, precipitates, and other inhomogeneous distributions of atoms in solids during irradiation. Studies of: (1) neutron and gamma irradiation effects on alloy microstructure and embrittlement, (2) freely-migrating and cascade defects, (3) irradiation performance of advanced nuclear fuels, (4) solid state amorphization, (5) radiation-induced segregation to internal and external defect sinks, (6) radiation-enhanced diffusion.
(7) inert-gases in solids, (8) surface modification and sputtering of alloys by ion bombardment, (9) in-situ studies of irradiation effects in the Intermediate and High-Voltage Electron Microscopes, and (10) 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.

33. TRIBOLOGICAL INVESTIGATION OF BORIC ACID BOUNDARY FILMS FORMING ON AL SURFACES
A. Erdemir, G. R. Fenske
(630) 252-5190 01-5 $87,000

Experimental investigation of boundary lubrication and chemical bonding mechanisms of boric-acid films on aluminum and aluminum alloys. Mechanisms of boundary film formation between aluminum surfaces and boric acid, to elucidate their fundamental tribological mechanisms under a wide range of contact pressures and shear rates using standard and micro-tribology test rigs. Thin boron-rich (e.g., boron, boron-oxides, and boric-acid) films deposited by dry (powder and PVD) and aqueous processes are characterized by surface analytical techniques (e.g., Auger, XPS, and NEXAFS) to determine the nature of the chemical bonding to aluminum and aluminum alloys. The effects of environment (e.g. humidity), temperature, stress, and chemistry on friction and chemical bonding are evaluated using macro- and nanotribometers in an effort to improve the metal-forming properties of lightweight materials.

34. CERAMIC MATERIALS
K. E. Gray, K. C. Goretta, D. J. Miller,
A. P. Paulikas, B. W. Veal Jr.
(630) 252-5525 01-5 $756,000

This program studies oxide ceramic materials, with the primary emphases on high-T_c superconductors and coatings. Synergistic efforts incorporating synthesis, characterization, fabrication are coupled to a wide range of fundamental electronic and structural properties. Materials engineering issues that limit performance and processing flexibility are also studied. The properties of ceramic protective coatings for use in high temperature corrosive environments (e.g., for high-temperature gas turbines) are studied. The single thallium layer HTS compounds are studied for use in powder-in-tube and coatings, because of their superior flux pinning. This program participates in the focus project on Mechanically Reliable Surface Oxides for Corrosion Resistance of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

Solid State Physics - 02 -

B. D. Dunlap - (630) 252-4925
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35. NEUTRON AND X-RAY SCATTERING
J. D. Jorgensen, G. P. Felcher, R. Osborn, D. L. Price
(630) 252-5513 02-1 $1,273,000

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

36. MAGNETIC FILMS
S. D. Bader, E. E. Fullerton,
M. Grimsditch
(630) 252-4960 02-2 $738,000

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

37. TAILORED PERMANENT MAGNETS
S. D. Bader
(630) 252-4960 02-2 $412,000

This program involves exploration for new and improved permanent magnets with high energy products. The approach is to utilize thin-film deposition techniques for fabrication, and magnetometry and electron microscopy for magnetic and structural characterizations, respectively. Rare-earth transition-metal binaries and ternary nitrides are being grown epitaxially via sputtering, and Nd-Fe-B is being grown via molecular beam epitaxy. Efforts are also being taken to interleave hard and soft ferromagnets on the nanometer-scale in order to test the new concepts of "exchange hardening" of permanent magnets. This should reduce rare-earth content, and theefore improve corrosion resistance and lower materials costs. Significant advances are possible technologically with new permanent magnets for energy applications.

38. SUPERCONDUCTIVITY AND MAGNETISM
G. W. Crabtree, W. K. Kwok, V. Vinokur, U. Welp
(630) 252-5509 02-2 $932,000

Experimental and theoretical investigations of the magnetic and superconducting properties of materials. Strong emphasis is being placed on studies of vortex matter in the mixed state of superconductors. Other programs include studies of the electronic properties of organic superconductors, heavy fermion and other narrow-band materials containing rare-earth and actinide elements. Experimental techniques include the transport and magnetic measurements, electron tunneling, magneto-optical imaging, de Haas-van Alphen effect, materials preparation and characterization. We maintain a strong theoretical effort emphasizing analytical theory and advanced numerical simulations.

39. SYNCHROTRON X-RAY SCATTERING
P. A. Montano, M. Bedzyk,
J. C. Campuzano, G. B. Stephenson,
H. You
(630) 252-6239 02-2 $716,000

X-ray scattering techniques, X-ray standing waves, glancing incidence fluorescence, X-ray absorption spectroscopy and resonant reflectivity have been used to characterize the structure and composition profile of epitaxially grown metals and multilayers. X-ray scattering has been utilized to characterize in-situ the growth mode of metallic thin films on different substrates. X-ray standing waves are being used to investigate surface, thin film and interface structures. Angle resolved photoemission has been employed to measure the electronic structure of high temperature superconductors. A new beamline for energy dispersive X-ray absorption measurements is being utilized for the study of transition metal magnetic alloys with emphasis on the use of magnetic circular dichroism. X-ray absorption technique used to study the structure of photoexcited states in molecules and crystals.

40. ADVANCED MATERIALS CHARACTERIZATION
P. A. Montano, M. A. Beno, G. Jennings, G. S. Knapp
(630) 252-6239 02-2 $825,000

Development of beamlines and instrumentation for the Basic Energy Sciences Synchrotron Radiation Center (BESSRC) at the Advanced Photon Source. A high brilliance source will be used to study the structure of new materials with particular emphasis in high energy X-ray scattering. Inelastic X-ray scattering is being used to study the momentum distribution of the electrons in solids. A new monochromator for high heat loads has been developed to use at the new beamlines. A new device, the elliptical multipole wiggler will be used to study the magnetic properties of materials.

41. CERAMIC EPITAXY FILMS AND COMPOSITES
D. Wolf, O. Auciello, C. Foster
(630) 252-5205 02-2 $292,000

Experimental research program on the processing, characterization, and property determination of single-crystal and polycrystalline epitaxial ceramic-oxide films and layered composites prepared by metal-organic chemical vapor deposition (MOCVD) techniques. The main objectives are twofold, namely (a) to enhance our fundamental understanding of the processing-structure-property relationship of thin ceramic films and multilayers synthesized by MOCVD and (b) to measure tensor properties in single-crystalline films, thus elucidating the performance of these materials. The main emphasis is on electro-ceramic materials, such as TiO_2, SnO_2, $PbTiO_3$, $SrTiO_3$, $BaTiO_3$, $PbZrO_3$, Y_2O_3, and $LiTaO_3$. Properties of interest involve their dielectric, piezoelectric, electro-optic, acousto-optic and elastic behavior.

42. CONDENSED MATTER THEORY
A. A. Abrikosov
(630) 252-5482 02-3 $858,000

Theory of superconductivity; electronic band structure, many-body effects; properties of low-dimensional systems; magnetic materials. Physical properties of superconductivity in heavy-fermion and high-T_c materials including anisotropic energy gap, nature of the pairing, vortex lattice, angular resolved photoemission, paramagnetic Meissner effect, superconductor-insulator transition, normal state anomalies. Theory of magnetic Compton scattering. Magnetic coupling in superlattice systems.

43. EMERGING MATERIALS
K. E. Gray, D. G. Hinks, D. J. Miller, J. F. Mitchell
(630) 252-5525 02-5 $532,000

This program includes materials engineering research and fundamental studies of new materials with a primary emphasis on superconductors. Sample fabrication includes single crystals and film depositions. Microcharacterizations, including electron microscopy and in-situ X-ray probes, are used as crucial links between physical properties and syntheses/processing. Studies seek to identify intrinsic potential of important new materials and the effects of extrinsic defects.

Materials Chemistry - 03 -

B. D. Dunlap - (630) 252-4924
Fax: (630) 252-4798

44. CHEMICAL AND ELECTRONIC STRUCTURE
J. M. Williams, U. Geiser, A. M. Kini, J. A. Schlueter, H. H. Wang
(630) 252-3464 03-1 $1,122,000

New materials synthesis and characterization focusing on synthetic organic metals and superconductors based on BEDT-TTF bis(ethylenedithio)tetrathiafulvalene, and various newly-synthesized organic electron-donor and electron-acceptor molecules. Development of structure-property relationships coupled with electrical and superconducting properties measurements. Development of improved crystal growth techniques. Phase transition and crystal structure studies as a function of temperature (10-300K) by use of the IPNS-single crystal diffractometer and a low-temperature (10 K) single crystal X-ray diffraction instrument. Co-development arrangements with Lake Shore Cryotronics, ["beta" test site for prototype llow-temperature (1.2 K to 298 K) AC susceptometer for magnetic properties measurements in applied magnetic fields] and Siemens International (Center of Excellence in X-ray scattering studies at ANL, and "beta" testsite for software development), by use of the new Siemens SMARTR diffraction system.

45. INTERFACIAL MATERIALS CHEMISTRY
A. R. Krauss, L. A. Curtiss, L. Iton
(630) 252-3520 03-2 $350,000

Basic research on interfacial phenomena is carried out in twoforefront scientific fields of materials science: (1) molecular sieve materials and their application in heterogeneous catalysis and (2) thin-film growth phenomena and film properties, with emphasis on mulitphase and multicomponent materials. The role of organic template molecules in the crystallization mechanisms of aluminosilicate zeolites. The application of modified zeolites and metallaluminophosphate materials as cayalysts in hydrocarbon oxidation reactions. Use of molecular sieve materials as matrices for the generation of intercrystalline particles and polymers, constrained in size and dimensionality. Computer simulations of framework and adsorbate molecular dynamics, as well as ab initio molecular oribital calculations of chemical properties of zeolite catalysts and template effects in microporous structure development. Growth mechanisms in multicomponent oxide thin films are being studied in situ utilizing pulsed ion beam surface analytical methods. Principal attention is focused on surface and interfacial properties, segregation mechanisms and nucleatoin/growth issues in ferroelectric and high temperature superconducting oxide materials. Nanocyrstalline diamond thin films with unique morphological, tribological and electrical properties are being produced by a new growth process utilizing $Ar\text{-}C_{60}$,$Ar\text{-}CH_4$, and $Ar\text{-}CH_4\text{-}N_2$ microwave enhanced chemical vapor deposition. Films procduced by these processes are being developed for low friction, long-lived rotating components and large area electron emitting structures.

46. AQUEOUS CORROSION
Z. Nagy, L. A. Curtiss, C. A. Melendres, R. M. Yonco
(630) 252-4355 03-2 $498,000

Basic research aimed at elucidating fundamental aspects of interfacial phenomena that occur on the surface of metals immersed in aqueous media under conditions relevant to light water fission reactors, nuclear waste storage environments, and the operation of batteries. 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 transient electrochemical techniques and in situ synchrotron adsorption radiation scattering methods. In situ characterization of electrochemical interfaces using synchrotron radiation techniques (X-ray and far infrared). Investigations of the key features of the interfacial chemistry associated with passivation processes (including charge transfer kinetics) using pulsed galvanostatic, potentiostatic, dc polarization, and ac impedance. A parallel computational effort seeks to simulate solid/liquid interface phenomena through the application of molecular dynamics methods combined with ab initio molecular orbital theory.

47. DYNAMICS, ENERGETICS AND STRUCTURE OR ORDERED AND METASTABLE MATERIALS
M.-L. Saboungi, L. A. Curtiss
(630) 252-4341 03-2 $284,000

Ordering is an important phenomenon in tailoring key properties that are significantly and technologically important in non-crystalline materials. In some liquid semiconducting alloys which exhibit a dramatic metal-non-metal (MNM) transition as a function of composition, ordering results from charge transfer. Our investigation of the structure, dynamics and electronic properties of liquid Zintl alloys has revealed unusual semiconducting behavior due to the presence in the liquid of complex anions. Room temperature molten salts continue to be investigated not only to understand the stability of the different ionic species but also to explore their effect on the potential use of these materials as electrolytes in high-energy batteries and in aluminum electroplating processes on steel. A combination of NMR, Raman spectroscopy, neutron diffraction and inelastic scattering measurements and ab initio calculations are used to determine their properties. New and powerful quantum mechanical techniques are being developed for application to various areas of materials chemistry including zeolites, silicon, clusters, gallium halides and Zintl molecules.

48. DIRECTED ENERGY INTERACTIONS WITH SURFACES
D. M. Gruen, W. F. Calaway, A. R. Krauss, M. J. Pellin
(630) 252-3513 03-3 $857,000

Development of multiphoton resonance and femtosecond short pulse ionization methods combined with sophisticated 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) sub-micron imaging mass spectrometry using laser desorption and sputtering,

(3) trace analysis for selected systems such as impurities in semiconductors, (4) isotopic studies of naturally occurring materials for study of environmentally-important problems anomalies. In a separate project, the composition and structure of thin films and solid surfaces are studied by ion beam scattering and direct recoil spectroscopy methods as well as conventional surface analysis methods such as Auger, UV and X-ray photoelectron spectroscopies, and secondary ion mass spectroscopy. Ion beam scattering and direct recoil methods permit characterization of thin film surfaces during deposition in ambient hydrogen, oxygen or nitrogen background gases. The system is being applied to the study of growth mechanisms in ferroelectric materials, high temperature superconductors and diamond thin films, where it is used to study transient and kinetically-dependent phenomena during deposition.

49. MOLECULAR IDENTIFICATION FOR SURFACE ANALYSIS

D. M. Gruen, K. R. Lykke, M. J. Pellin
(630) 252-3513 03-3 $345,000

Surface analysis of the molecular composition of complex solids using Fourier transform ion cyclotron resonance mass spectroscopy coupled with resonant, ponderomotive, and "soft" laser ionization methods. The solid surfaces to be investigated include conducting polymers, plastics, fullerenes, 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 self assembled monolayer (SAM) compounds.

Facility Operations - 04-

D. Moncton - (630) 252-7950
Fax: (630) 252-4599

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50. APS USER TECHNICAL AND ADMINISTRATIVE INTERFACE

S. Barr, S. Davey, G. K. Shenoy
(630) 252-5537 04-1 $2,800,000

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

51. INTENSE PULSED NEUTRON SOURCE PROGRAM

B. S. Brown, J. M. Carpenter, C.-K. Loong, G. E. McMichael, W. G. Ruzicka
(630) 252-4999 04-1 $10,112,000

Operation and development of IPNS, a pulsed spallation neutron source for condensed matter research with neutron scattering techniques. The facility is equipped with 11 instruments which are regularly scheduled for users and 3 instruments under development. The facility has been run since 1981 as a national facility in which experiments are selected on the basis of scientific merit by a nationally constituted Program Committee. Approximately 350 experiments, involving about 200 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., ALCAN, Texaco, Corning, General Electric, Amoco, BP Chemicals) and is encouraged. Relevant Argonne research programs appear under the neutron activities of the Materials Science Division of Argonne National Laboratory.

52. ASD R&D IN SUPPORT OF OPERATIONS

E. Crosbie, R. Damm, J. Galayda, M. Knott, R. Kustom, A. Lumpkin, G. Mavrogenes, L. Teng, M. White
(630) 252-7796 04-1 $4,200,000

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

53. APS ACCELERATOR OPERATION AND SUPPORT
J. N. Galayda, L. E. Temple
(630) 252-7796 04-1 $47,178,000

The APS accelerator systems are designed and operated to meet very challenging reliability and availability goals for providing X-ray beams to teams of APS research users. These goals were established to be consistent with the considerable value of the time and effort expended by the community of X-ray experimenters to prepare and complete their experiments. Development of sophisticated software tools to automate supervisory and troubleshooting functions are vital to achieving high levels of reliability and availability during scheduled operations. Administrative and support functions that insure regulatory compliance and required utility services and maintenance of critical support systems are also included.

54. XFD R&D IN SUPPORT OF OPERATIONS
E. Gluskin, T. Kuzay, D. M. Mills, G. K. Shenoy
(630) 252-5537 04-1 $15,855,000

The R&D needed to support user operation at the APS will optimize X-ray source and beamline capabilities. These studies will examine operating characteristics of X-ray source and beamline components with the goal of improving their performance. Activities include studies of novel X-ray sources, and engineering of beamline front ends, beamline optics and instruments. The influence of higher power loads from X-ray flux produced by new and novel insertion devices, and higher stored currents on the beamline components will be evaluated. In support of users, software based on EPICS to control the beamlines will be developed and tested. New synchrotron techniques will be developed which will lead to newer user scientific capabilities.

55. APS EXPERIMENTAL FACILITIES OPERATION
J. Hawkins, M. Ramanathan, T. Rauchas, G. K. Shenoy
(630) 252-5537 04-1 $5,845,000

To establish a smooth transition between the construction of beamlines of the APS and the user operations phase, the facilities operations group was established. This group has full responsibility for APS beamline operation, and for the maintenance and trouble shooting of insertion devices, beamline front ends, personnel safety systems, and radiation shielding. All systems will be optimized to achieve desired operational performance in support of the APS users.

BROOKHAVEN NATIONAL LABORATORY
Upton, NY 11973

D. McWhan - (516) 344-3927
Fax: (516) 344-2918

Metallurgy and Ceramics - 01 -

D. O. Welch - (516) 344-3517
Fax: (516) 344-4071

56. THEORY OF ALLOY PHASES
M. Weinert, M. Alatalo, P. Allen (SUNY-Stony Brook), M. Sluiter, R. E. Watson
(516) 344-2684 01-1 $243,000

Theoretical studies of complex alloy phases using first-principles electronic structure methods. Microstructure and phase stability of complex multicomponent metallic systems and their relationships to phase diagrams. Relative stability of ordered alloys and the structural properties of metals. Defects, impurities, low concentration ternary alloys, and impurity/clustering interactions. Effects of configurational and vibrational entropy. Development of new techniques for the calculation of the properties of materials, combined use of electronic structure and statistical mechanics calculations.

57. NANOSCALE STRUCTURE AND STRUCTURAL DEFECTS IN ADVANCED MATERIALS
Y. Zhu, B. Nielsen
(516) 344-3057 01-1 $277,000

The main goal of this program is to study nanoscale structure and structural defects and their role in determining the properties of technologically-important materials such as superconductors, magnets, semiconductors, and corrosion-resistant metal oxides. The techniques used are primarily transmission electron microscopy (TEM) and positron annihilation spectroscopy (PAS). Computer simulations, theoretical calculations, and modeling are done to aid in the interpretation of experimental data. Quantitative studies of charge distributions, grain boundaries, interfaces, and other structural defects are made using advanced TEM methods of electron diffraction, imaging, and spectroscopy. Positron methods are used to study secondary defect formation in Si, ion beam surface melted and resolidified materials, ion-implanted polymer, impurity-vacancy complexes, and Si nanocrystals in SiO_2.

58. MECHANISMS OF METAL-ENVIRONMENT INTERACTIONS
H. S. Isaacs, L. Oblonsky
(516) 344-4516 01-2 $405,000

Studies of the properties, formation, and breakdown of passive and anodically grown oxide films on metals and alloys. Surface morphology and atomic structure using atomic force and tunneling microscopy. Concentrations and valency of elements in surface oxides using X-ray absorption. Growth and reduction processes in passive 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 simulating localized corrosion. Structure of the electrolytes, salt film formation, and electromigration. This program participates in the focus project on Bulk Metallic Glasses of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

59. SUPERCONDUCTING MATERIALS AND BASIC MATERIALS SCIENCE OF HIGH-T_C CONDUCTOR FABRICATION
M. Suenaga, Z.-X. Cai, Q. Li,
A. R. Moodenbaugh, D. O. Welch,
Y. Zhu
(516) 344-3518 01-3 $1,434,000

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.

Solid State Physics - 02 -

S. M. Shapiro - (516) 344-38822
Fax: (516) 344-2918

60. NEUTRON SCATTERING
J. D. Axe, W. Bao, S. M. Shapiro,
G. Shirane, J. M. Tranquada, P. Wochner, A. Zheludev
(516) 344-3821 02-1 $1,721,000

The principal objective is the study of fundamental interactions in solids by elastic and inelastic neutron scattering. The phenomena studied include structural and magnetic phase transformations, magnetic structure, and elementary excitations such as spin-waves and phonons. Current specific topics of interest include high-temperature superconductivity, as well as normal state properties of cuprate superconductors and related systems (e.g., nicklates) with highly correlated d-electrons. Of particular interest is the interplay between electronic, structural and magnetic degrees of freedom in these systems, as well as in f-electron heavy fermion systems. The effect of spatial dimensionality on magnetic properties is a long-standing and ongoing activity. Present work is concerned with S=1 linear chain antiferromagnets with Haldane singlet ground states, and S= 1/2 structures with unusual magnetic order (spin dimers, spin ladders, etc.). Continuing studies of Martensitic transformations which show unusual temperature dependent phonon behavior

61. POWDER DIFFRACTION
D. E. Cox, T. Iglesias, T. Vogt,
P. M. Woodward
(516) 344-3818 02-2 $233,000

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 giant magnetoresistive maganites. Phase transition studies at high and low temperatures, including magnetic ordering. High pressure and low temperature studies in diamond--anvil cells by synchrotron X-ray diffraction techniques with monochromatic radiation. Development of instrumentation and software for powder diffraction analysis. Synthesis and characterization of complex oxide systems.

62. X-RAY DIFFRACTION
D. Gibbs, E. Dimasi, J. P. Hill, B. Ocko, T. Thurston, H. Zajong
(516) 344-4608 02-2 $994,000

The objective of this program is to use the techniques of synchrotron X-ray scattering to study basic structural, electronic, and magnetic properties of condensed matter systems. The X-ray scattering group, as members of three participating research teams, operates and maintains three X-ray beamlines at the National Synchrotron Light Source (X22A, X22B, and X22C). Particular emphasis is placed on investigations of surface and interfacial phenomena, on the structure and magnetic spectroscopy of magnetically ordered crystals and on electronic excitations in solids. Current examples of projects include: 1) the study of metal surface and overlayer phase transformations in UHV, 2) the study of electrochemically driven surface and overlayer, reconstructions at metal/electrolyte interfaces, including liquid metal surfaces, 3) the study of fluctuations at liquid surfaces and interfaces, 4) X-ray magnetic scattering studies of bulk and surface rare earths, transition elements, and actinides, and 5) inelastic X-ray scattering studies of electron excitations in light metals. The X-ray group is also an active member of the Complex Materials CAT constructing beamlines at the Advanced Photon Source.

63. POSITRON SPECTROSCOPY
B. Nielsen, P. Asoka-Kumar
(516) 344-3525 02-2 $780,000

Perfect and imperfect solids, solid heterostructures and interfaces, and their surfaces are investigated using variable energy positron beams (0.1 eV - 3 MeV). A high intensity positron beam that utilizes a copper isotope produced with the High Flux Beam Reactor has become fully operational and can deliver a beam of peak intensity $1x10^8$e+/s. The beam has been used to probe the structure of the technologically important SiO_2-Si interfaces. Current interests, utilizing a continuous source, involved the study of the durability of paint and coating systems, the role of defects in thermal aging process, and the light induced degradation of amorphous Si. An exciting new development is the elemental specificity of the positron annihilation spectra which allows one to chemically "fingerprint" the first neighbor of a vacancy.

64. CONDENSED MATTER THEORY
V. J. Emery, M. Blume, S. Maslov, V. N. Muthukumar, R. E. Watson, M. Weinert
(516) 344-3765 02-3 $701,000

Solid state theory including nonlinear systems, theory of correlated electron systems, especially charge transport and superconductivity in synthetic oxides. Theory of alloys including heats of formation, using local density functional theory. Electronic structure of metallic surfaces. Applications to X-ray and neutron scattering, and to photoemission.

65. X-RAY MICROSCOPY BEAMLINE UPGRADE
J. Kirz
(516) 344-5601 02-4 $115,000

The X1A Undulator Beamline at NSLS originally designed to feed two experimental stations from a single monochromator of moderate resolution. Since then, the combination of microscopy with spectroscopy has become a particularly powerful tool. To do spectroscopy on both stations simultaneously, the beamline was redesigned with separate monochromators for the two stations providing the opportunity to upgrade the optics, to improve the resolution of both monochromators, and to improve the resolution/flux trade-off. The design and performance is being documented. This X-ray spectro-microscopy capability is used to examine materials structures and biological specimens.

66. PRECISION PHOTO-FABRICATION USING X-RAYS
E. D. Johnson, D. P. Siddons
(516) 344-4603 02-5 $200,000

The NSLS X-ray ring is used as a source of hard (E>15 keV) X-rays to extend lithographic exposure techniques to the length scale of centimeters. The properties of the source also make it possible to fabricate fully three dimensional structures while maintaining micrometer precision. The objectives of this project are to provide tools for utilizing this resource and conduct research defining optimal operating parameters for exposures in various configurations. Precision patterning over large areas with aspect ratios exceeding 100:1 and the fabrication of re-entrant three dimensional objects in resist have been demonstrated. Scanning systems and mask writing equipment matched to the requirements of hard X-ray exposures have been developed. Current research is aimed at providing a better understanding between the resist properties, exposure parameters, and device geometry to develop design rules for high quality precision fabrication in this high aspect ratio regime. Development of the next generation exposure station is also under way.

67. ELECTRON SPECTROSCOPY
P. D. Johnson, D. Bosov, A. Federov,
P. Henning, C. Homes, M. Strongin,
T. Valla
(516) 344-3705 02-5 $1,036,000

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, Photoemission, Inverse Photoemission, Spin Polarized Photoemission, and infrared spectroscopy. The major part of the program is supported by beamlines at the NSLS. These include both conventional monochromators and the more advanced spherical grating monochromators used on the undulator sources. The latter devices are dedicated to the spin polarized photoemission components of the program. Ongoing research includes: (a) photoemission and inverse photoemission studies of the electronic structure of metal overlayers, clean metal surfaces, and adsorbate covered surfaces; (b) studies of surface and thin film magnetism and the effect of adsorption on surface magnetism; (c) studies of the spin dependent electronic structure in magnetic quantum well. An infrared program has been initiated on charge transport in complex materials, including organic conductors, high-T_c superconductors, doped fullerene systems and other unusual metals. It is anticipated that the complex conductivity will show unique features due to the breakdown on the usual quasiparticle picture in these materials.

68. STRUCTURE-SENSITIVE PROPERTIES OF ADVANCED PERMANENT MAGNET MATERIALS: EXPERIMENT AND THEORY
D. O. Welch, L. H. Lewis
(516) 344-3517 02-5 $523,000

It the task of this program to study the basic relationships between crystal lattice defects and the microstructure of advanced high-coercivity permanent magnet materials and their macroscopic magnetic properties, such as coercivity, remanence, and maximum energy product, which are relevant to their energy related technological application. The research features both theory and experiment, including the use of the National Synchrotron Light Source (NSLS), and features a collaboration between researchers from Brookhaven National Laboratory (BNL), industry (primarily Magnequench International, Inc. and Rhone-Poulenc, Inc.) other national laboratories [Idaho National Engineering and Environmental Laboratory (INEEL), and Ames Laboratory] and universities (primarily Lehigh University and Carnegie-Mellon University). This program is part of the focused project on Tailored Microstructures in Hard Magnets of the Department of Energy (DOE) Center of Excellence for the Synthesis and Processing of Advanced Materials.

Materials Chemistry - 03 -

69. NEUTRON SCATTERING - SYNTHESIS AND STRUCTURE
J. Z. Larese
(516) 344-4349 03-1 $504,000

Neutron and X-ray scattering techniques are used to investigate phase transitions and critical phenomena of atomic and molecular films adsorbed on surfaces. Efforts are focused on a characterization of the structure and dynamics of molecular and rare gas films adsorbed on metal oxide, graphite and boron nitride surfaces. Additional work includes the synthesis and characterization of unique, high-quality single-crystal materials with novel physical and chemical properties, the development of devices to perform state-of-the-art, automated experiments and molecular simulations of surface films. This effort is also responsible for the operation and maintenance of multipurpose neutron and X-ray beamlines are available for use by the outside scientific community.

70. SYNTHESIS AND STRUCTURES OF NEW CONDUCTING POLYMERS J. McBreen
(516) 344-4513 03-2 $403,000

Development of a fundamental understanding of ionically and electronically conducting polymers and development of techniques for tailoring the materials with highly specific electrical and optical properties. Research consists of the synthesis of new conducting polymers and the exploration of their physical and chemical properties with a number of spectroscopic techniques, including electrochemistry, X-ray absorption spectroscopy, X-ray diffraction, positron annihilation, Fourier transform infrared spectroscopy, Raman spectroscopy and electrical resistivity measurements. The materials of interest are linear polyethers, polysiloxanes, polypyrroles and polythiophenes. The materials are chemically modified by the covalent attachment of electrically active side groups or by introducing polar plasticizers or anion complexing agents. This is a collaborative program between

Brookhaven National Laboratory, Polytechnic University, and Power Conversion, Inc.

Facility Operations - 04 -

71. OPERATIONS OF NSLS
M. Hart, J. Hastings, R. Heese, J. Keane, R. Klaffky, S. Kramer, S. Krinsky, W. Thomlinson
(516) 344-4966 04-1 $17,288,000

This program supports the operation of the National Synchrotron Light Source, which is a large user facility devoted to the production and utilization of synchrotron radiation. 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 beamlines on the vacuum ultraviolet (VUV), and X-ray storage rings. As this is the first facility in the U.S. that was designed expressly for the use of synchrotron radiation, there are extensive development programs to improve the stability, reliability, and lifetime of electron beams and to develop new insertion devices which give even brighter photon beams. Equally important are programs to develop new beamline instrumentation including beamline optics, monochromators and detectors which will permit users to take full advantage of the unique research capabilities offered by the NSLS. The PRTs continue to invest heavily in the facility, and the program seeks to keep the facility at the forefront to justify this investment.

72. HIGH FLUX BEAM REACTOR
D. Rorer, J. Barkwill, W. Brynda, J. Carelli, C. Dimino, S. Golden, R. Karol, D. Ports, A. Queirolo, L. Somma
(516) 344-4056 04-1 $22,134,000

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, 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.

IDAHO NATIONAL ENGINEERING AND ENVIRONMENTAL LABORATORY
P. O. Box 1625
Idaho Falls, ID 83415

A. Denison - (208) 526-8135
Fax: (208) 526-5327

Metallurgy and Ceramics - 01 -

A. Denison - (208) 526-8135
Fax: (208) 526-5327

73. STRESS DISTRIBUTION IN GRADED MICROSTRUCTURES
B. H. Rabin
(208) 526-0058 01-5 $339,000

Develop fundamental understanding of the effects of microstructure, processing conditions, and specimen geometry on the thermomechanical behavior of graded materials. Fabrication of two-phase coatings and bulk materials with controlled microstructural gradients and varying geometries by ion-beam assisted deposition (IBAD) and powder metallurgy techniques. Focus on model materials systems in which significant property mismatch exists between components, e.g. AL_2O_3/Ni. Thermophysical and mechanical property characterization of graded composites. Mapping of residual stresses by X-ray and neutron diffraction methods, and florescence spectroscopy. Comparison of experimental results with predictions from elastic-plastic finite element method (FEM) modeling of stress distributions. Use of FEM models to design gradient material microstructures for severe service conditions. This program participates in the focus projects on Hard Magnets and on Materials Joining of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

74. ROLE OF IMPURITIES IN MICROSTRUCTURAL EVOLUTION OF RAPIDLY SOLIDIFIED MATERIAL
R. N. Wright
(208) 526-6127 01-5 $235,000

Examination of phenomena associated with the interaction of low levels of impurities with quenched-in defects in rapidly solidified metals. Interactions studies in simple systems to determine fundamental mechanisms. Initial studies of high-purity aluminum and aluminum doped with ppm levels of lead or indium containing ion-implanted helium have shown accelerated helium bubble growth when liquid precipitates are attached to bubbles. Rapidly quenched, high-purity aluminum and dilute aluminum alloys containing substitutional elements with different vacancy binding energies, as well as carbon as an interstitial impurity, have been examined. The transformation from a dendritic as-solidified structure to equiaxed grains during isothermal annealing and with superimposed plastic strain is being studied in detail for Ag-2% Al and Ni-Cu alloys. Solute redistribution by a moving grain boundary is modeled. This program participates in the focus project on Mechanically Reliable Surface Oxides for High Temperature Corrosion Resistance and Polymers of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

UNIVERSITY OF ILLINOIS FREDERICK SEITZ MRL

104 S. Goodwin Avenue
Urbana, IL 61801

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

Metallurgy and Ceramics - 01 -

75. TRANSPORT PROCESSES IN LOCALIZED CORROSION
R. C. Alkire
(217) 333-0034 01-1 $196,060

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

76. DEFECTS, DIFFUSION, AND NON-EQUILIBRIUM PROCESSING OF MATERIALS
R. S. Averback
(217) 333-4302 01-1 $244,446

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.

77. MOLECULAR SPECTROSCOPY OF THE SOLID-LIQUID INTERFACE
P. W. Bohn
(217) 333-0676 01-1 $147,026

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.

78. CENTER FOR MICROANALYSIS OF MATERIALS
J. A. Eades
(217) 333-8396 01-1 $803,000

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

79. DIFFRACTION AND MICROSCOPY FROM SURFACES
J. A. Eades
(217) 333-8396 01-1 $70,880

Electron diffraction and electron microscopy are used for the study of surfaces. Reflection high-energy electron diffraction (RHEED) and low-energy diffraction (LEEM) are studied in conventional and convergent-team mode. The emphasis is an technique development.

80. ATOMISTICS OF GROWTH AND TRANSPORT AT METAL AND SEMICONDUCTOR INTERFACES
G. Eulich
(217) 333-6448 01-1 $129,308

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.

81. ATOMIC RESOLUTION ELECTROCHEMISTRY OF CORROSION AND DEPOSITION PROCESSES
A. A. Gewirth
(217) 333-8329 01-1 $142,510

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

82. TRANSMISSION ELECTRON MICROSCOPY OF SURFACES AND INTERFACES
J. M. Gibson
(217) 333-2997 01-1 $186,406

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.

83. CRYSTAL GROWTH AND PHYSICAL PROPERTIES OF METASTABLE SEMICONDUCTING, CERAMIC AND METALLIC ALLOYS
J. E. Greene
(217) 333-0747 01-1 $239,882

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.

84. SURFACE AND INTERFACE X-RAY DIFFRACTION
I. K. Robinson
(217) 244-2949 01-1 $176,858

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

85. OPTICAL CHARACTERIZATION OF NOVEL MATERIALS AND DEVICES
J. O. White
(217) 333-8876 01-1 $70,880

Development of novel optical methods for materials characterization. Spectroscopy combined with near-field scanning optical microscopy. Optical properties of quantum defined structures. Quantum point contacts studied at THz frequencies. Time resolved nonlinear spectroscopies.

86. ORGANIZATION OF THE SINGLE-CRYSTAL SOLID-LIQUID INTERFACE: ENERGIES, STRUCTURES AND ELECTRONIC SYNERGISM
A. Wieckowski
(217) 333-7943 01-1 $154,699

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

87. MICROSTRUCTURE EVOLUTION, INTERFACES AND PROPERTIES IN STRUCTURAL CERAMIC COMPOSITES
A. Zangvil
(217) 333-6829 01-1 $167,760

Phase and microstructural evolution in structural ceramics and ceramic matrix composites; SiC-based solid solutions; nitride, boride and mullite-based systems; interfaces and fracture toughness. Oxidation mechanisms of ceramic matrix composites; theoretical model of particle oxidation in an oxide matrix.

88. SOLUTE EFFECTS ON MECHANICAL PROPERTIES OF GRAIN BOUNDARIES
H. K. Birnbaum, I. Robertson
(217) 333-1370 01-2 $265,885

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. This program participates in the focus projects on Metal Forming of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

89. COUNCIL ON MATERIALS SCIENCE
C. P. Flynn
(217) 333-1370 01-2 $100,851

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.

90. CHEMICAL VAPOR DEPOSITION OF METAL AND CERAMIC THIN FILMS
G. S. Girolami
(217) 333-2729 01-2 $77,056

Synthesis of thin film metals and ceramics by chemical vapor deposition method at low temperature. Studies of the chemistry of precursor compounds at solid surfaces. Development and investigation of surface-selective chemical vapor deposition methods. Preparation of transition metals and their carbide, boride and nitride binary phases using MOCVD methods. Characterization of the microstructures, chemistry, electronic structure, physical properties of the films using a variety of methods.

91. HIGH TEMPERATURE MECHANICAL BEHAVIOR OF CERAMICS
D. F. Socie
(217) 333-7630 01-2 $64,454

Behavior of engineering materials subjected to 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.

92. MICROSTRUCTURE BASED CONTINUUM MODELING OF THE MECHANICAL BEHAVIOR OF MATERIALS
P. Sofronis
(217) 333-2636 01-2 $83,810

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

93. STRUCTURE AND KINETICS OF INTERFACES IN NON-EQUILIBRIUM MATERIALS
P. Bellon
(217) 333-0284 01-3 $62,990

Develop basic understanding of the behavior of interfaces in systems far from equilibrium. Interface behavior in presence of external forcing functions such as irradiation, plastic deformation, etc. Kinetic roughening and atomic mixing. Experiments and computer simulations.

94. DEVELOPMENT OF X-RAY SYNCHROTRON INSTRUMENTS
H. K. Birnbaum
(217) 333-1370 01-3 $379,456

Design, development and fabrication of X-ray beamline equipment for the UniCat sector at the Advanced Photon Source located at Argonne National Laboratory. Program is interactive with Oak Ridge National Laboratory, National Institute of Science and Technology and UOP Corporation.

95. STRUCTURE AND KINETICS OF ORDERING TRANSFORMATIONS IN METAL ALLOYS AND SILICIDE THIN FILMS
H. Chen
(217) 333-7636 01-3 $112,026

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.

96. MATERIALS CHEMISTRY OF OXIDES CERAMICS; FIELD RESPONSIVE ORGANIC INCLUSION COMPLEXES
W. G. Klemperer
(217) 333-2995 01-3 $131,038

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.

97. SYNTHESIS AND PROPERTIES OF ELECTRICAL CERAMICS

D. A. Payne
(217) 333-2937 01-3 $186,602

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.

98. ATOMIC SCALE MECHANISMS OF VAPOR PHASE CRYSTAL GROWTH

A. Rockett
(217) 333-0417 01-3 $68,647

Atomic dynamics on semiconductor surfaces during growth from the vapor phase; photoelectron spectroscopic characterization of the energy band structure, near surface chemistry, and interactions between thin films; dielectrics for Si-Ge and compound semiconductors; and characterization of reactions to form contact metallizations for microelectronic integrated circuits.

99. MAGNETIC BEHAVIOR OF NANOPHASE MATERIALS

M. B. Salamon
(217) 333-6186 01-3 $96,653

Experimental and theoretical studies of the magnetic properties of nanophase metals and mixtures of metals. Interfacial effects of magnetic particles embedded in non-magnetic matrices. Investigation of spin waves, quantum tunneling of the macroscopic magnetization of particles and macroscopic quantum coherence effects. This program participates in the focus projects on Nanostructural Materials of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

100. FERROELECTRIC THIN FILMS

D. Viehland
(217) 333-6837 01-3 $91,739

An interlaboratory collaboration to explore the effects of epitaxy on the properties of ferroelectric materials. Based on advanced methods for the synthesis of ferroelectrics by molecular beam epitaxy at ORNL and by sol gel methods at Illinois. Studies by X-ray scattering, Z-contrast electron microscopy, and low energy electron microscopy. Dielectric characterization to measure polarizibility, hysteresis and piezoelectric deformations on a 1 um length scale.

101. PROCESSING OF MONODISPERSE CERAMIC POWDERS

C. Zukoski
(217) 333-7379 01-3 $114,874

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.

102. MICROSCOPIC PROCESSES IN IRRADIATED CRYSTALS

R. S. Averback, C. P. Flynn
(217) 333-4302 01-4 $143,329

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

103. RADIATION EFFECTS IN METALS AND SEMICONDUCTORS

I. M. Robertson
(217) 333-6776 01-4 $90,671

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.

104. THE RATIONAL DESIGN OF CHIRAL ZEOLITES
S. E. Denmark
(217) 333-0066 01-5 $61,928

Templated growth of zeolites containing chiral pores and voids. Design of organic amines and ammonia salts to serve as templates for hydrothermal growth.

105. MOLECULAR PRECURSOR ROUTE TO NANOPOROUS SOLIDS
J. S. Moore
(217) 244-4024 01-5 $78,817

Synthesis of multi-topic ligands designed to spontaneously organize into nanoporous coordination networks. Structure and property characterization. Development of constitutive models to understand crystal packing and enhance rational design of new materials.

Solid State Physics - 02 -

106. MICROSCOPIC MECHANISMS OF CRYSTAL GROWTH
D. Cahill
(217) 333-6753 02-2 $74,453

Fundamental studies of vapor phase crystal growth. Use of scanning tunneling microscopy to quantify the evolution of surface morphology during epitaxial growth of pure elements and alloys and the effects of low-energy ion bombardment on morphology and microstructure.

107. ELECTRONIC PROPERTIES OF SEMICONDUCTOR SURFACES AND INTERFACES
T.-C. Chiang
(217) 333-2593 02-2 $174,058

Synchrotron radiation photoemission X-ray diffraction, and STM studies of the electronic properties atomic structure, and growth behaviors of semiconductor surfaces and interfaces prepared in situ by molecular beam epitaxy and chemical vapor deposition; properties and atomic structure of alloy surfaces.

108. OPTICAL SPECTROSCOPIES OF NOVEL MAGNETIC SYSTEMS
S. L. Cooper
(217) 333-2589 02-2 $56,818

Infrared, optical reflectivity and inelastic scattering methods used to study phase transitions and low frequency excitation spectra of magnetic systems. Correlation-gap semiconductors. Giant magnetoresistance compounds.

109. GROWTH AND PROPERTIES OF NOVEL MBE MATERIALS
C. P. Flynn
(217) 244-6297 02-2 $163,906

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

110. CHARGE TRANSPORT ACROSS SUPERCONDUCTOR-SEMICONDUCTOR INTERFACES
L. H. Greene, P. M. Goldbart,
D. Van Harlingen
(217) 333-7315 02-2 $424,826

A coordinated experimental and theoretical study of the static and dynamic properties of hydride superconductor-semiconductor structures. Electronic transport, superconductive tunneling, and magnetization measurements are conducted in planar microfabricated structures of high-quality niobium thin films grown directly on III-V semiconductors to study the superconducting proximity effect and Andreev reflection.

111. THEORY OF SOLIDS, SURFACES AND HETEROSTRUCTURES
R. M. Martin
(217) 333-4229 02-2 $75,185

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

112. SEMICONDUCTOR/INSULATOR STRUCTURES
H. Morkoc
(217) 333-0722 02-2 $107,568

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

113. DESIGN AND SYNTHESIS OF NEW ORGANOMETALLIC MATERIALS
T. B. Rauchfuss
(217) 333-7355 02-2 $120,098

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

114. MICROSCOPIC THEORIES OF THE STRUCTURE AND PHASE TRANSITIONS OF POLYMERIC MATERIALS
K. S. Schweizer
(217) 333-6440 02-2 $61,830

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

115. PROPERTIES OF CRYSTALLINE AND LIQUID CONDENSED GASES
R. O. Simmons
(217) 333-4170 02-2 $120,530

Measurement and theory of momentum density in bcc, hcp, and liquid helium, in solid neon and argon, and molecular solids, pulsed neutron scattering, electronic and phonon excitations in solid helium-three by inelastic X-ray scattering, thermal and isotopic defects in helium crystals, quantum effects in diffusion.

116. NUCLEAR MAGNETIC RESONANCE IN SOLIDS
C. P. Slichter
(217) 333-3834 02-2 $201,740

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.

117. ELECTRO-ACTIVE AND NONLINEAR OPTICAL POLYMERS
S. I. Stupp
(217) 333-4436 02-2 $133,161

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.

118. METALLOPORPHYRINS AS FIELD RESPONSIVE MATERIALS
K. S. Suslick
(217) 333-2794 02-2 $62,797

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.

119. CARRIER TRANSPORT IN QUANTUM WELLS - PICOSECOND IMAGING
J. P. Wolfe
(217) 333-2374 02-2 $81,079

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

Materials Chemistry - 03 -

120. HIGH PRESSURE STUDIES OF MOLECULAR AND ELECTRONIC PHENOMENA
H. G. Drickamer
(217) 333-0025 03-1 $143,367

Use of high pressure to study electronic phenomena with emphasis on tuning of triplet energy levels in molecules containing N and O atoms in rigid polymeric media and on understanding changes in physical and chemical properties important for molecular electronic devices.

121. MECHANISTIC AND SYNTHETIC STUDIES IN CHEMICAL VAPOR DEPOSITION
R. G. Nuzzo
(217) 244-0809 03-3 $74,641

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.

122. OPTICAL SPECTROSCOPY OF SURFACE PROCESSES IN THIN FILM DEPOSITION
E. G. Seebauer
(217) 333-4402 03-3 $62,313

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

LAWRENCE BERKELEY NATIONAL LABORATORY

1 Cyclotron Road
Berkeley, CA 94720

D. S. Chemla - (510) 486-4999
Fax: (510) 486-7768

Metallurgy and Ceramics - 01 -

123. NATIONAL CENTER FOR ELECTRON MICROSCOPY
U. Dahmen
(510) 486-4627 01-1 $2,438,000

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

124. CRYSTALLOGRAPHY OF MICROSTRUCTURES
U. Dahmen
(510) 486-4627 01-1 $158,000

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.

125. STRUCTURE AND PROPERTIES OF TRANSFORMATION INTERFACES
R. Gronsky
(510) 486-5674 01-1 $93,000

Relationship between atomic structure of homophase or heterophase boundaries and their properties, with attention to the solid state reactions that they either initiate, catalyze or propagate. Atomic resolution imaging, spatially-resolved diffraction, and spatially-resolved spectroscopy for location and identity of atomic species. Electron microscopy. Computer simulation of microstructural development and characterization methodologies for enhanced interpretation of results. Object-oriented code development. Engineering of new materials through control of atomic structure.

126. THIN FILMS, COATINGS AND NANOSTRUCTURES
K. Krishnan
(510) 486-4614 01-1 $107,000

The goals of this research are the synthesis and characterization of atomically-engineered thin films with novel magnetic, optical, and electrical properties. Fundamental investigations of new phenomena as well as the development, control and optimization of microstructures to achieve enhanced properties will be stressed. In addition to synthesis and property measurement, development of nanoscale spectroscopic, imaging and diffraction methods at the appropriate level of resolution, with either electron or photon probes, will be critical to the success of these investigations and hence will be an integral part of these research projects. Of current interest in this program are the synthesis and understanding of metallic, oxide/nitride magnetic thin films and nanostructures with novel anisotropy, coupling, hysteretic and transport behavior, evolution and control of microstructures to optimize these properties, application of magnetic measurements for nondestructive evaluation of materials and the electron emissivity of diamond thin films.

127. CAM HIGH PERFORMANCE METALS PROGRAM
J. W. Morris, Jr., D. C. Chrzan,
R. O. Ritchie, G. Thomas
(510) 486-6482 01-2 $538,000

This CAM program focuses on advanced metallic materials of interest to American industry. It includes fundamental research on microstructure and mechanical behavior and specific investigations of interesting metallic systems. It is organized in three projects: (1) Mechanical Behavior, which addresses the mechanisms of creep, fatigue and fracture, friction and wear. (2) Advanced Metals, which concentrates on the understanding and use of functional instabilities in the understanding and development of modern alloys, such as eutectic alloys for low-temperature bonding, controlled elongation alloys for formability, and electromagnetic field effects, and (3) Hard Magnets, which attempts to predict magnetic properties based on microstructural parameters such as grain size, phase distribution and texture, and design processing schemes to achieve superior microstructure and properties. This program participates in the focus projects on Metal Forming and on Tailored Microstructures in Hard Magnets of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

128. CAM CERAMIC SCIENCE PROGRAM
L. C. DeJonghe, R. Cannon, A. Glaeser,
W. Moberlychan, R. Ritchie, G. Thomas, A. Tomsia
(510) 486-6138 01-3 $1,143,000

The CAM Ceramic Science Program has three linked objectives: the development of predictive, quantitative theories of densification and microstructure development in heterogeneous powder compacts, the application of these theories to produce advanced structural ceramics with improved performance beyond 1900 K, and the evaluation of the mechanical properties of these ceramics, at temperatures above 1700 K. It develops model experiments that facilitate investigation of fundamental aspects of microstructural development and processing, and their application of model ceramic systems. It develops models and means for initial powder compact structural control including the production and use of coated powders; it examines the microstructural evolution and control during densification in relation to interface properties; it produces particulate ceramic composites based on SiC, and it tests mechanical properties of such ceramics in particular high temperature creep and fatigue; it characterizes micro- and nano-chemistry and structure in relation to high temperature mechanical and environmental performance; it addresses issues in ceramic/ceramic and ceramic/metal joining.

129. CAM ELECTRONIC MATERIALS PROGRAM
E. Haller, J. Ager III, E. Bourret,
Z. Liliental, W. Walukiewicz,
J. Washburn, E. Weber,
K. M. Yu
(510) 486-5294 01-3 $1,009,000

Research in this program focuses on an improved understanding of the materials science of artificially structured semiconductor and semiconductor-metal systems with special emphasis on wide band gap materials. Basic studies concentrate on the relationships between synthesis and processing conditions and the properties of semiconductor materials, as modified by the resulting structural and electronic imperfections. Growth of compound semiconductors by metalorganic epitaxies is combined with detail studies of structural and electronic properties of thin films and interfaces. Extensive transmission electron microscopy investigations of the nature and origin of defects at interfaces and within epitaxial layers closely correlated with electrical measurements on the same specimens provide feedback to the crystal growth synthesis and processing work at Berkeley and at other National Laboratories. Optical spectroscopies ranging from the near UV to the far infrared region of the electromagnetic spectrum, electron paramagnetic resonance spectroscopy and electrical transport measurements often in combination with cryogenic temperatures and/or large hydrostatic pressures give the complementary electronic properties. Theoretical and experimental work on the effects of atomic scale diffusion and the differences between solid solubility limits of dopants and the maximum concentration of free carriers is pursued. Novel types of processing methods including annealing under large hydrostatic pressures and with tunable synchrotron radiation, to increase the electrically active fraction of dopants, are explored. Progress in this area is applicable to the design of advanced photovoltaic energy conversion devices, solid state light sources, and of a large variety of sensors used in energy conversion, energy distribution and energy consumption. This program participates in the focus projects on Processing for Surface Hardness, and High Performance Photovoltaic Materials of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

130. NONDESTRUCTIVE CHARACTERIZATION TOOLS FOR ENERGY-EFFICIENT MANUFACTURING
J. W. Morris Jr., J. Clarke
(510) 486-6482 01-5 $189,000

The scanning SQUID microscope as a probative tool for the nondestructive characterization for engineering alloys, to enhance process and quality control for energy-efficient manufacturing. Addresses critical elements of microstructure that are not readily accessible by existing techniques including residual plastic deformation, mechanical degradation, internal precipitation, and thermal sensitization. The research team includes representatives of three distinct disciplines: (1) materials scientists on microstructure-property relations that determine engineering properties; (2) physicists in modern SQUID devices and techniques; (3) electron microscopists who can identify the magnetic phenomena that cause particular microstructural states to have characteristic magnetic signatures. Unique, high-T_c scanning SQUID microscope recently developed at LBNL to examine well-characterized metallurgical specimens. The SQUID signals will be interpreted through high-resolution studies of magnetic patterns, obtained through Lorentz imaging and SPLEEM analysis in the National Center for Electron Microscopy. The research should identify important problems for which SQUID microscopy is ideally suited, and other problems for which SQUID microscopy, while promising, is inapplicable or inherently noncompetitive with other techniques.

Solid State Physics - 02 -

131. QUANTUM SIZE EFFECTS IN SEMICONDUCTOR NANOSTRUCTURES
D. S. Chemla
(510) 486-4999 02-2 $254,000

A unique ultrashort optical pulse, high magnetic field, and low temperature facility will be exploited and methods for characterizing the phase and amplitude of polarization waves will be developed for exploring the ultrafast dynamics of materials with reduced dimensionality. The current research focuses on: (1) Effect of Magnetic Confinement on Optical Nonlinearities, and (2) Understanding Dissipation and Relaxation in the Quantum Kinetics Regime. The objective of this program is to explore the physical properties of material systems whose sizes, of the order of a few nanometers, are intermediate between that of atoms/molecules and that of bulk solids. Because of quantum size effects, the properties of such systems are size and shape dependent and not like those of atoms nor those of macroscopic solids. Because of the ultrasmall size of these systems, the dynamics of their electronic, vibronic and energy excitations is, in the femtosecond regime.

132. SUPERCONDUCTIVITY, SUPERCONDUCTING DEVICES, AND 1/F NOISE
J. Clarke
(510) 642-3069 02-2 $193,000

DC Superconducting QUantum Interference Devices (SQUIDs) used in a wide variety of measurements. An ultrasensitive SQUID spectrometer is used to detect nuclear magnetic resonance (NMR) and nuclear quadrupole resonance (NQR) in molecular solids in the frequency range below 1 MHz. The NMR signal from Xe has been greatly enhanced by Fermic exchange with optically pumped Rb, and observed at frequencies down to 200 Hz; this technique has been exploited to image frozen Xe at 12 kHz, the lowest frequency at which an NMR image has been observed. Other experiments include NQR of deuterium in deuterated materials, and two-dimensional NQR spectra. A SQUID is used to investigate low-frequency magnetic flux noise in high transition temperature (Tc) superconductors. These measurements are aimed at reducing the level of noise in SQUID magnetometers. Related experiments include measurements of the dynamics of flux vortices in two-dimensional arrays of Josephson junctions near the Kosterlitz-Thouless transition temperature. Experiments are performed to investigate he pairing symmetry in $YBa_2Cu_3O_{7-x}$ crystals by means of Josephson tunneling along the c-axis direction into lead films. The junctions are grown across a single twin boundary of the crystal, and the dependence of the critical current on a magnetic field in the plane of the junction is measured as a function of the angle between the field and the twin boundary. The results provide strong evidence fro mixed d- and s-wave pairing, with a reversal in the sign of the s-wave component across the twin boundary.

133. SURFACE, INTERFACE, AND NANOSTRUCTURE STUDIES USING SYNCHROTRON RADIATION IN COMBINATION WITH OTHER PROBES
C. S. Fadley
(510) 486-5774 02-2 $335,000

New synchrotron-radiation-based instrumentation and methods for studying solid surfaces, interfaces, and nanostructures have been developed. These methods together with other techniques such as scanning tunneling microscopy are being applied to systems of fundamental and technological interest. A principal interest is photoelectron spectroscopy, diffraction, and holography with ultrahigh resolutions in energy and angle. A photoelectron spectrometer/diffractometer with unique capabilities for use at the Advanced Light Source also was completed, and first experiments performed with it. This system provides the highest combined resolutions in energy (1 in 10^4) and angle ($\pm 1°$) currently available at the ALS. The beamline also covers a broad range of energies from 30 eV to 1500 eV, and permit variation of the polarization from linear to circular. Some of the first studies carried out with this system were full-solid-angle photoelectron angular distributions from oxide and element atoms for 0 on W(110), and spin-polarized photoelectron diffraction from antiferromagnetic MnO(001). Parallel theoretical work on spin-polarized photoelectron diffraction, circular dichroism in both non-magnetic and magnetic systems, and photoelectron holography also is continuing, with successful interpretations of experimental data for both spin-polarized photoelectron spectra and circular dichroism in photoelectron angular distributions.

134. ELECTRON TRANSPORT IN NANOSTRUCTURES
P. McEuen
(510) 486-6817 02-2 $94,000

Novel nanostructures using a combination of lithography and chemical synthesis, to probe their properties using local electrical measurements. Current work focuses on the electrical measurement of single metal and semiconductors clusters fabricated by colloidal synthesis. In one approach, and atomic force microscope (AFM) with a conducting tip will be employed to probe clusters bound to surfaces. In a second approach, clusters will be used to bridge lithography patterned electrodes. DC transport measurements of these systems will directly probe the single electron charging energies and quantum level spacing of these clusters. In addition to DC transport, photocurrent and ultrafast spectroscopy will also be performed. This work will be performed in collaboration with the research groups of Paul Alivisatos, Peter Schultz, John Clarke, Joe Orenstein, and Daniel Chemla. The goal is to use a multidisciplinary approach to probe and control the properties of materials on a nanometer scale.

135. LINEAR AND NONLINEAR TERAHERTZ SPECTROSCOPY OF MATERIALS
J. Orenstein
(510) 486-5880 02-2 $114,000

Focuses on the terahertz and far-infrared properties of materials. The terahertz region of the spectrum is of critical importance in the spectroscopy of condensed matter systems. Spin waves in magnets, superconducting band gaps, and transitions between quantum confined states of low-dimensional systems all fall in this range. In spite of its importance, terahertz spectroscopy has been hindered by the lack of suitable tools. Our group uses time-domain terahertz spectroscopy (THz-TDS), a new technique which has revolutionized far-infrared spectroscopy. THz-TDS is based on electron magnetic transients generated optoelectronically with the help of sub-picosecond laser pulses. These transients are single-cycle bursts of electromagnetic radiation whose spectral density spans the range from below 100 GHz to above 5 THz. By measuring the pulse shape after transmission through a sample, we obtain both the real and imaginary parts of the dielectric function, without the need for Kramers-Kronig analysis. In recent studies we have used this unique source to study the microwave properties of the vortex state the Josephson plasma resonance in anisotropic superconductors, nonlinear electrodynamics in high-T_c superconductors, and giant magnetoresistance in multilayer thin films.

136. FAR-INFRARED SPECTROSCOPY
P. L. Richards
(510) 486-3027 02-2 $149,000

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 single crystals of new high-T_c superconductors, measurements of nonlinear hopping conductivity in doped GE near the metal-insulator transition, and measurements of the far infrared spectra of carbon nanotubes. Improvements in infrared technology include: development of thin-film voltage biased superconducting bolometers for detecting infrared, and millimeter wave radiation. This novel approach promises orders of magnitude increase in detector speed and linearity for both high-T_c and low T_c bolometers.

137. UNENHANCED RAMAN SPECTROSCOPY OF MATERIALS AND SURFACES
G. Rosenblatt
(510) 486-6606 02-2 $5,000

Raman spectroscopy probes the atomic vibrations of a material and can yield important information about chemical, physical, and mechanical properties. Unique Raman instrumentation has been developed that has high sensitivity, a profiling and mapping capability with a spatial resolution of 5 um, and the ability to study adsorbed molecules and films (as thin as a monolayer) in-situ in an ultrahigh vacuum chamber. A variety of technologically important materials systems - including hard III-V semiconductors including nitrides, amorphous carbon films, chemically synthesized diamond films, reinforced and phase stabilitized ceramics, and polymers are to be investigated. Collaborative work with researchers in industry is leading to an improved understanding of the relationship between structure and mechanical performance of amorphous, "diamond-like" carbon films. Raman and photoluminescence are being used to obtain unique maps of strain distributions in semiconductor films, in ceramic composites, and in carbon-based films.

138. ELECTRODE SURFACE PROCESSING
P. Ross
(510) 486-6226 02-2 $283,000

Advanced plasma surface-modification and ion-implantation techniques are being used to modify battery and fuel cell electrodes. Plasma and ion-beam surface modification techniques of several different kinds will be employed including nitrogen-ion implantation, metal-ion implantation, and synthesis of thin-film surface layers that are atomically mixed into the electrode substrate. It is anticipated that surface-modified lithium electrodes will have significantly better stability, safety and lifetimes in nonaqueous battery electrolytes, compared to pure lithium electrodes. The goal is to replace commercially available lithium-carbon electrodes with metallic lithium, and thereby provide a significant increase in delivered energy and power per unit battery mass. Also, novel electrocatalyst structures will be formed using these techniques. It is anticipated that nonequilibrium multimetallic surfaces will exhibit unusual and enhanced electrocatalytic properties, compared to surfaces of the same elements prepared using conventional bulk synthetic methods.

139. STUDIES OF THE METAL/SOLUTION INTERFACE WITH X-RAYS

P. N. Ross
(510) 486-6226 02-2 $165,000

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 reflections parallel and perpendicular to the reflecting plane to obtain complete structural characterization of the interfacial region. Initial experiments directed towards 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). Recent experiments include determining lattice expansion accompanying hydrogen atom adsorption (from solution) on Pt, Ir and Pd surfaces, the 2D structure of halide ions on Pt, and the 2D structure of metals in the first stages of electrodeposition. Future experiments are 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.

140. FEMTOSECOND DYNAMICS IN CONDENSED MATTER

C. V. Shank
(510) 486-6557 02-2 $248,000

To further the basic understanding of ultrafast dynamic processes in condensed matter. Research efforts are 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. Measurement techniques which allow rapid events to be resolved with the unprecedented time resolution of a few femtoseconds. The generation and compression of femtosecond pulses has been extended to cover the entire visible spectrum from 400 to 800 nm, providing the capability to investigate a large variety of important materials. Ultrafast electron-hole dynamics in the highly confined semiconductor structures CdSe and InP nanocrystals and CdS/HgS nanocrystal onions. A novel three-pulse photon echo technique allows separation of the vibrational dynamics from the polarization dephasing process. Three-pulse photon echo measurements in InP indicate that electronic dephasing occurs on a 100 fs time scale at 15 K, with significant contributions from an acoustic phonon heatbath. Contributions from acoustic phonons dominate the dephasing at room temperature. These results are in good agreement with our previous measurements in CdSe. A partial dephasing at early times which results from a second excited state originating from valence band mixing is observed. This is a direct result of the quantum confinement. Three-pulse photon echo techniques are being applied to studies of electronic dephasing of oxazine molecules in an amorphous polymer host. Such measurements elucidate the coupling between a probe molecule and the host environment. The dephasing dynamics are consistent with a low-frequency phonon activated process. The polarization decay times vary from ~40fs at room temperature to ~160fs at 28 K. In addition, the dephasing dynamics appear to be strongly dependent on the molecular nature of the solute.

141. EXPERIMENTAL SOLID-STATE PHYSICS AND QUANTUM ELECTRONICS

Y. R. Shen
(510) 486-4856 02-2 $192,000

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 of all types.

142. SURFACE INSTRUMENTATION

Y. R. Shen
(510) 642-4856 02-2 $193,000

The surface instrumentation project develops new experimental techniques for the atomic and molecular scale characterization of surfaces. These include the scanning tunneling and atomic force microscopes (STM, AFM), nonlinear optical techniques of sum frequency and second harmonic generation (SFG, SHG), and surface crystallography by LEED. (This project is part of the CAM Surface Science and Catalysis Program).

143. TIME-RESOLVED SPECTROSCOPIES IN SOLIDS

P. Y. Yu
(510) 486-8087 02-2 $119,000

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, trapping of defects, phonon-phonon interactions, and electron-electron interactions. The experiments involve exciting dense electron-hole plasmas in bulk or nanostructured semiconductors and monitoring the time evolution of the electron and phonon distribution functions by Raman scattering and photoluminescence. Another area of investigation involves the study of properties of solids under high pressure.

144. QUANTUM THEORY OF MATERIALS
M. L. Cohen, S. G. Louie
(510) 486-4753 02-3 $291,000

Research to further basic understanding of the physical properties of materials and materials systems such as surfaces and interfaces. Emphasis on carrying out quantum-mechanical calculations on realistic systems so that a microscopic understanding may be obtained from first principles. Model systems are also examined, and new theoretical techniques are developed. Studies include bulk materials, high-T_c superconductors, fullerides, surface and chemisorbed systems, interfaces, materials under high pressure, clusters, and defects in solids. Close collaboration with experimentalists is maintained and comparisons with experiment show that the calculations are accurate and of predictive power. Bulk materials research is focused on: electronic, magnetic, structural, and vibrational properties; crystal-structure determination; solid-solid phase transformations at high pressure; and defect properties. Surface and interface research focused on atomic, electronic, and magnetic structures. Superconductivity research is focused on mechanisms for high transition temperature and possibilities of superconductivity at high pressures.

145. CENTER FOR X-RAY OPTICS
D. Attwood
(510) 486-4463 02-4 $2,023,000

The Center for X-ray Optics (CXRO) pursues advances in X-ray optics and the use of modern sources of radiation. Emphasis is placed on the use of soft X-rays and extreme ultraviolet (EUV) radiation, a spectral region characterized by photon energies extending from below 100 eV to as high as 10 keV, and wavelengths extending from 0.1 nm to 20 nm. Activities in the past year have included soft X-ray microscopy for the physical and life sciences, with spatial resolution well below 100 nm (nanometers), a microprobe for X-ray fluorescence and diffraction studies of widely varying samples, generally permitting subpicogram elemental analysis on a 1 micron spatial scale in the presence of a high-Z host. There has also been considerable work done on bendable mirrors for EUV microfocusing applications, such a micro-ESCA and micro-XANES. With support from the microelectronics industry, a unique at-wavelength EUV interferometer has been constructed, using coherent radiation from the Advanced Light Source (ALS), to measure the surface figure of multilayer coated optics for eventual use in a potential nanoelectronic manufacturing plant. Deep etch X-ray lithography (LIGA) was also used at the ALS to fabricate micron sized mechanical parts for use in precision manufacturing and to support research. New capabilities for absolute metrology and calibrations at EUV and soft X-ray wavelengths were used to characterize scattering and reflectivity from EUV multilayer mirrors. There has also been activity on the theory of scattering at EUV wavelengths at the ALS. We continue to use the existing five CXRO beamlines at the ALS for the above pursuits. A long sought a state-of-the-art electron beam pattern writer, the "Nanowriter," has been installed a centerpiece of a new nanofabrication facility. The facility has just been commissioned, enabling the fabrication of significantly improved diffractive X-ray optics, structures for surface materials science, quantum electronic devices, and using it's unique stitching accuracy, complex mask structures for nanoelectronic lithography applications.

146. CAM HIGH-T_C SUPERCONDUCTIVITY PROGRAM
A. Zettl, J. Clarke, N. E. Phillips,
P. Richards
(510) 642-4939 02-5 $440,000

Studies in three areas: basic science, thin films and their applications, and electron microscopy. Basic science 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. Includes theoretical work, the synthesis of new materials, growth of single crystals, and measurement of physical properties (including magnetic susceptibility, transport properties, specific heat, isotope effects, mechanical properties, nonlinear electrodynamics, microwave absorption, terahertz spectroscopy, electron tunneling, and infrared absorption). Includes first principles calculations and model-based interpretations of measured properties. Thin-films and applications research includes fabrication and processing. Investigation of physical and electrical properties, development of thin-film devices, including SQUIDS and other applications of Josephson devices, and bolometric radiation sensors. The electron microscopy research 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. Fullerene materials are also synthesized and explored by electron microscopy and transport measurements and theory. This program participates in the focus projects on Hard Magnets and Photovoltaics of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

Materials Chemistry - 03 -

147. LOW-TEMPERATURE PROPERTIES OF MATERIALS
N. E. Phillips
(510) 486-4855 03-1 $125,000

Measurements of low-temperature properties of materials, particularly superconductors, to contribute to the general understanding of materials properties and structure-property relations. The emphasis is on specific heat measurements (5mK to 130K; pressures to 20kbar; magnetic fields to 10T), but the electrical resistivity and magnetic susceptibility are also measured in cases of interest. Current investigations are mainly on high-T_c oxide superconductors and heavy-fermion compounds. The measurements on oxide superconductors give fundamental information on the nature and mechanism of the superconductivity and the mechanism of vortex pinning, and technically useful information on the volume fraction of superconductivity and its relation to synthetic procedures; those on heavy-fermion compounds give information on the interrelation of superconductivity and magnetism.

148. CAM BIOMOLECULAR MATERIALS PROGRAM
M. D. Alper, C. Bertozzi, D. Charych, J. F. Kirsch, D. E. Koshland, Jr., P. G. Schultz, R. Stevens, C.-H. Wong
(510) 486-6581 03-2 $538,000

The goal of this program is the use of natural biological concepts, processes, structures, and molecules as the basis for the synthesis of new materials. One component focuses on the use of natural, engineered and "created" enzymes to catalyze synthetic reactions. The unique sterochemical control exerted by enzymes and their ability to catalyze reactions at low temperature allows the synthesis of materials with structures and properties that cannot be achieved using conventional synthetic routes. Efforts on the design of reaction conditions, engineering of enzyme structure and activity, generation of catalytic antibodies for materials synthesis. Other polymers with structures inspired by biological polymers are being synthesized chemically. Work also on the synthesis of organic thin films which mimic the biological membrane. Membranes self-assemble, present defined and controllable surfaces, detect the presence or absence of specific materials. These properties are exploited to alter interfacial and surface properties and to fabricate sensor devices. Thin film sensors have been developed to detect influenza virus, botulism E.coli and cholera toxins and small molecules, e.g., glucose. Similar films have been used to direct the ordered crystallization of inorganic salts. Research is also focused on the modification of the surface of materials to improve their biocompatibility. *Funded jointly by DOE's Division of Materials Sciences and Energy Biosciences.

149. CAM POLYMERS AND COMPOSITES PROGRAM
M. M. Denn, A. Chakraborty, D. Gin, S. Muller, J. Reimer, D. Theodorou
(510) 486-0176 03-2 $580,000

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

150. ATOMIC LEVEL STUDIES OF TRIBOLOGICAL PROPERTIES OF SURFACES AND LUBRICANTS
M. Salmeron
(510) 486-6230 03-2 $451,000

Understanding of the basic physical and chemical processes that govern the tribological properties of surfaces (adhesion, friction and wear) and to determine the role of surface films of lubricants in modifying these tribological properties. The atomic structure of surfaces and the mechanical properties of adhesion and friction at point contacts are studied with the Scanning Tunneling Microscope (STM) and the Atomic Force Microscope

(AFM). These techniques allow the study of the substrate atomic structure and that of the adsorbate before and after contact. A Surface Force Apparatus (SFA) is used in combination with Second Harmonic and Sum Frequency Generation to study the conformation (orientation) and vibrational properties of monomolecular films in-situ, during compressive and shear stresses. Studies employ simple model lubricants including atomic adsorbates (O, C, S, etc.), simple organic molecules, and long chain hydrocarbons (alkylsilanes, perfluorinated hydrocarbons) that can form self-assembled monolayers covalently bonded to various surfaces. A new, non-contact AFM is used to study liquid films and their wetting, spreading and reactions with substrates, with a few tens of nanometer resolution.

151. SEMICONDUCTOR THIN FILMS USING NANOCRYSTAL PRECURSORS
P. Alivisatos
(510) 643-7371 03-3 $130,000

Methods have been developed to prepare high quality monodisperse, nanometer size crystallites of many common semiconductors. Investigations the phase of diagram of these nanocrystals. They melt at lower temperatures than the bulk solid, and that they transform to denser phases at higher pressures than the bulk. These nanocrystals can be bound to metal surfaces using self-assembled monolayers. Investigations of the use of these surface-bound nanocrystals as low temperature precursors to thin films. This program participates in the focus project on Nanoscale Materials of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

152. NUCLEAR MAGNETIC RESONANCE
A. Pines
(510) 486-6097 03-3 $708,000

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 and experimental approaches. Some developments currently underway in this direction are iterative and multiple-pulse sequences, geometric quantum phase, multiple-quantum NMR, zero-field and SQUID-NMR, double-rotation NMR, NMR imaging of structure and flow, optical pumping and surface-enhanced NMR. The second direction involves the application of novel NMR methods and instrumentation to materials research. The developments above are being used, for example, to study surfaces, clusters and nanostructures, semiconductors, superconductors, silicates, zeolites, catalysts, liquid crystals, polymers, bipolymers and glasses.

153. CAM SURFACE SCIENCE AND CATALYSIS PROGRAM
G. A. Somorjai, M. B. Salmeron,
Y. R. Shen, M. A. Van Hove
(510) 486-4831 03-3 $898,000

Surface instrumentation development is an important part of this project. The Surface Science effort includes studies of the atomic role surface structure of solids and adsorbs monolayers. Metal single crystal surfaces (Pt, Pd, Rh), single crystal thin films grown by vapor phase epitaxy (Fe_3O_4, MgC_{12}, NaCl, ice) and metal nano-cluster arrays (Pt, Ag) in the 2.5 nm - 100 nm size range produced by electron beam lithography on various oxides (SiO_2, Al_2O_3, TiO_2) are utilized in this investigation. The adsorbates are organic molecular (ethylene, benzene...). The techniques used in these studies are low energy electron diffraction-surface crystallography (LEED), scanning microscopies (STM and AFM), sum frequency generation (SFG) vibrational spectroscopy and electron microscopy. Catalysis research is focussed on studies of catalysts during reaction, in-situ, using STM, SFG, and UV-Raman and correlating the microscopic kinetic parameters (turnover rates, schistion energies) with the molecular surface structure and composition. Hydrocarbon conversion reaction (hydrogenation, dehydrogenation, isomerization, polymerization, hydrogenolysis, hydrodechlorization), combustion of alkones (methane, ethane) and carbon monoxide are studied. Model catalysts (single crystals, nano-cluster arrays, thin films) of plutonium and its bimetallic alloys, rhodium pollodium and silver are utilized in most of the studies. Tribology studies of the mechanical properties of surfaces (adhesion, friction, lubrication) focus on polymers (Polyethylene, polypropylene) and hard carbon (diamond-like) coatings. AFM, the surface force apparatus and SFG permit correlation of friction, elastic modules and hardness with surface structure, crystallinity and lubricant bondings.

154. SYNTHESIS OF NOVEL SOLIDS
A. M. Stacy
(510) 642-3450 03-3 $45,000

Research on new synthetic procedures for the preparation of advanced materials with potentially useful electronic and/or magnetic properties. Current research is focused in three project areas: 1) Precipitation of oxide superconductors from ionic liquids; 2) Preparation and characterization of new layered niobium oxide superconductors; and 3) Investigation of cooperative interactions in rare earth transition metal phosphides. The structure and properties of the materials that are synthesized are determined in order to correlate synthesis and properties, as well as structure and properties.

155. SURFACE THEORY
M. A. Van Hove
(510) 486-6160 03-3 $69,000

This project develops theoretical methods for the analysis of surfaces and interfaces, in particular for structure determination by various electron scattering, diffraction and tunneling techniques. The project operates in particularly close collaboration with experimental and computational programs at LBNL. Many of the theoretical methods developed in this project are of particular importance for a host of experimental techniques that will be employed by users of LBNL's Advanced Light Source. The project also manages a database of solved surface structures. The Surface Structure Database (SSD) is marketed world-wide to provide the detailed atomic-scale structures of surfaces determined from experiment.

156. STIMULATED DESORPTION OF HALOGENS FROM SURFACES
J. A. Yarmoff
(909) 787-5336 03-3 $15,000

Desorption induced by electronic transitions (DIET) is used to investigate the interaction of radiation with surfaces. In our work, we monitor the ions produced by core-level excitation. Of particular interest are chemical systems with applications in the processing of semiconductor devices and in environmental management. Synchrotron radiation-based techniques, e.g., soft X-ray photoelectron spectroscopy (SXPS) and photon stimulated desorption (PSD), are performed at the National Synchrotron Light Source, Brookhaven National Laboratory, at the Advanced Light Source (ALS), and at MAX-lab in Lund, Sweden. From this work, a model of the halogen/semiconductor etching process, based on the CaF_2/Si(111) interface provided information on the formation of F-center defects in ionic solids. In addition, at the University of California, Riverside, studies of surface damage induced via electron stimulated desorption (ESD) are performed. Recent studies have concentrated on using ESD to probe ion-surface interactions. Currently, we are modeling the reduction of selenite, a contaminant found in groundwater, by investigating the interaction of SeF_6 with Fe surfaces.

Facility Operations - 04 -

157. ADVANCED LIGHT SOURCE OPERATIONS
D. Chemla
(510) 486-4999 04-1 $27,466,000

The Advanced Light Source (ALS) at the Lawrence Berkeley National Laboratory (LBNL) delivers X-rays and vacuum ultraviolet light of unprecedented brightness to users from a wide range of disciplines in industry, academia, and government laboratories. Facility construction was completed in March 1993. First light was seen in October 1993, and new beamlines have been installed at a steady pace since then. Five undulator beamlines and six bend-magnet beamlines, some serving multiple experimental stations, were operational in 1996. These numbers will almost double to nine and 11, respectively, by 1998. Highlights of the scientific program include: (1) Several ALS groups are using X-ray "spectromicroscopes" that combine imaging with high-resolution spectroscopy to obtain chemical, structural, or magnetic information from tiny features, such as those on semiconductor microchips and high-density magnetic data-storage media, as well as polymers and advanced composite materials; (2) The technique of soft X-ray fluorescences spectroscopy has become a powerful new method that complements existing techniques for the investigation of both fundamental and applied problems in the electronic structure of materials, surfaces, molecules adsorbed on surfaces, and interfaces buried beneath surfaces; (3) High-resolution photoemission techniques, including photoelectron diffraction, photoelectron holography, and resonant photoemission, are providing detailed information about the electronic and atomic structure of materials and surfaces; (4) The combination of synchrotron radiation with molecular beams and lasers is a opening new window into the fundamentals of chemical-reaction dynamics, including those processes of importance for combustion and atmospheric pollution; (5) Ultrahigh-resolution photoelectron and photoionization data are enhancing the ability of researchers to understand the fundamental behavior of electrons in atoms, especially electron-electron correlation, a problem of basic importance in molecules and solids, as well. In addition to research activities, the ALS has a vigorous outreach program to local industry. Research program under way include microelectronics (Intel and others), magnetic materials (IBM, which is also a major partner in one of the undulator beamlines), and polymers (Dow Chemical). In early 1997, a new protein crystallography beamline will open with the support and participation of biotech firms.

LAWRENCE LIVERMORE NATIONAL LABORATORY

P.O. Box 808
Livermore, CA 94550

L. Newkirk - (510) 422-5476
Fax: (510) 424-2252

Metallurgy and Ceramics - 01 -

158. EFFECT OF IMPURITIES, FLAWS AND INCLUSIONS ON ADHESION AND BONDING AT INTERNAL INTERFACES

W. E. King, G. Campbell, S. M. Foiles, D. Medlin, W. G. Wolfer
(510) 422-6547 01-2 $251,000

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 Al and Cu and the effect of impurities such as Cu and Ag. Interface structure calculations using state-of-the-art interatomic potentials. Bicrystals for experimental studies fabricated using ultra high vacuum diffusion bonding. Determination of interface atomic structure using quantitative high resolution electron microscopy. This program participates in the focus project on Design and Synthesis of Ultrahigh-Temperature Intermetallics of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

159. THE KINETICS OF PHASE TRANSFORMATIONS IN THE HEAT AFFECTED ZONE OF WELDS A COMBINED IN-SITU EXPERIMENTAL INVESTIGATION WITH NUMERICAL MODELING

J. W. Elmer, J. Wong
(510) 422-6543 01-5 $370,000

This research program addresses the fundamental issue of microstructural evolution that occurs under highly non-isothermal conditions by solid state phase transformations during the processing of materials by welding. Although welding is an enabling technology used in many industrial settings, it is least understood in terms of the phases that actually exist, the variation of their spatial disposition with time, and the rate of transformation from one phase to another at various thermal coordinates in the vicinity of the weld. In this research, we apply two unique experimental tools developed at LLNL: a spatially resolved X-ray diffraction (SRXRD) method to determine the phases present and map out spatially their relative fraction in both the heat affected zone (HAZ) in fusion welds; and a time-resolved X-ray absorption spectroscopic (TRXAS) technique to directly determine the rate of transformation of one phase to the other in-situ under the highly non-isothermal conditions that persist during welding. Direct observation of HAZ phase transformations will be made initially on two material systems: a commercially pure titanium that exhibits an allotropic transformation from a hcp phase to a bcc phase upon heating, and a two-phase stainless steel alloy that exhibits an austenitic (fcc) to ferritic (bcc) phase transformation upon heating. A central goal of this project is to utilize the in-situ phase and real-time transformation kinetic data to help develop a generalized model of HAZ phase transformation behavior, and to verify this model for allotropic and two-phase transformation behavior. This program participates in the focus project on Materials Joining and Mechanically Reliable Surface Oxides for High Temperature Corrosion Resistance of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

160. ROLES OF INTERFACES AND INTERPHASES ON SUPERPLASTICITY IN CERAMICS

T. G. Nieh, L. Hsiung, J. Wang
(510) 422-9802 01-5 $869,000

Research program focused on developing a basic understanding of the effects of interfacial chemistry, structure, and the presence of different phases, in particular thin films, on the sliding properties of an interface. Fabrication of metallic and ceramic bicrystals with controlled orientations and interfaces using the LLNL diffusion bonding machine. Characterization of interfacial cohesion, structure, and other mechanical properties. Effects of liquid film to be studied using quartz bicrystal interleaved with a B_2O_3 layer. Study of superplasticity in composites. Theoretical approach to incorporate ab initio total energy methods and molecular dynamics simulations. This program participates in the focus project on Metals Forming and Processing for Surface Hardness of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

Solid State Physics - 02 -

161. SCIENCE OF THIN FILMS AND CLUSTERS
L. L Chase, A. V. Hamza, A. Van Buren
(510) 422-6151 02-2 $334,000

The electronic and geometric structures of surfaces, interfaces and ultrathin films constructed from nanocyrstalline clusters. A combination of unique synthesis methods and powerful characterization techniques are used to study nanoscale properties, such as quantum confinement, and to address issues like grain boundary effects and structure-property relationships in nanophase systems. Characterization methods include photoelectron spectroscopies, EXAFS, X-ray diffraction, scanning tunneling and atomic force microscopy, TEM, and small angle electron scattering. The evolution of properties as a function of particle size from the nanoscopic to macroscopic scale will be used to develop a strategy for the preparation and utilization of novel assemblies of clusters. Materials and processes studied include oxidation of Si and other semiconductors and the deposition of insulating or semiconducting thin films and ion-implanted layers.

162. OPTICAL MATERIALS RESEARCH
S. A. Payne, C. D. Marshall, R. H. Page,
K. Shaffers
(510) 422-0570 02-2 $251,000

Linear and nonlinear optical properties of optical materials are investigated including behavior at high laser intensities and during ultrashort pulses of light. Properties measured and modeled include absorption and emission spectra and cross sections, lifetimes of optical excitations, and nonlinear transmission and propagation effects. 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.

Materials Chemistry - 03 -

163. INVESTIGATION OF NANOSCALE MAGNETICS
J. G. Tobin
(510) 422-7247 03-1 $463,000

Integrated experimental-theoretical investigation of magnetic structure-property relationships at the nanometer level. Focus on restricted dimensional systems such as surfaces, interfaces, and ultrathin films in arrangements such as epitaxially-deposited monolayer, bi-layer, and tri-layer films and multilayers. Experiments use novel magnetic double polarization measurements with circularly polarized synchrotron radiation combined with spin polarized electron detection. Theory applies spin-specific multiple scattering simulations. Investigations will permit the direct determination of atomically-local magnetic and geometric structure.

164. GROWTH AND FORMATION OF ADVANCED HETEROINTERFACES
L. J. Terminello, R. Hill, I. Jimenez,
S. Kakar, J. Klepeis, R. Treusch
(510) 422-7956 03-2 $453,000

Microscopic investigation of solid heterointerfacial growth and formation. Experimental determination of evolution of the atomic geometry and electronic structure during initial stages of interface formation. Studying interfaces such as SiC/Si(100) and other atomic layer epitaxies with nanometer or smaller domains. Utilizes synchrotron-based probes such as photoelectron holography, X-ray fluorescence, multiple angle, valence-band and core-level photoemission, and near-edge core level photoabsorption to investigate heterojunctions. Experimental results are compared with theoretical models of atomic and electronic structure using ab initio molecular dynamic simulation from self consistent interatomic forces.

LOS ALAMOS NATIONAL LABORATORY

Los Alamos, NM 87545

D. M. Parkin - (505) 667-9243
Fax: (505) 665-2992

Metallurgy and Ceramics - 01 -

165. UNIFIED THEORY OF EVOLVING MICROSTRUCTURES
R. Lesar, E. A. Holm
(505) 665-0420 01-1 $447,000

Fundamental theory and modeling of microstructural evolution, combining materials modeling techniques to bridge length scales from the atomistic to the microstructural. Atomistic simulations are being used to examine grain-boundary mobility, dislocation interactions with grain boundaries, etc. Dislocation-dynamics simulations to examine the role of dislocation microstructural evolution in the presence of moving grain boundaries. Information from the atomistic and dislocation dynamics incorporated into more accurate, three-dimensional, Potts model simulations of grain growth, recrystallization, and other dynamic phenomena. Application of the modeling to aluminum and other materials for which there is data on dislocation dynamics, annealing of dislocation structures, dynamic recrystallization, etc.

166. THEORY AND DESIGN OF MONOLITHIC AND DUAL PHASE ALLOYS
D. J. Thoma, R. C. Albers, S. P. Chen, F. Chu, C. L. Fu, C. T. Liu, T. E. Mitchell, J. Wills, M. Yoo
(505) 665-3645 01-2 $289,000

Improve Laves phase toughness and ductility. Understanding of defect structure and deformation mechanisms. Electronic and geometric contributions to phase stability and alloying behavior. Dual phase (Laves/bcc) structures. Experimental and theoretical alloy design methodologies to elucidate deformation mechanisms.

167. NEUTRON IRRADIATION INDUCED METASTABLE STRUCTURES
K. E. Sickafus, M. Nastasi, R. B. Schwarz
(505) 665-3457 01-4 $643,000

Irradiation phenomena and damage microstructures in single and polycrystalline ceramic compounds exposed to neutrons, ions, and electrons. Radiation tolerant and radiation resistant ceramics such as $MgAl_2O_4$ spinel and cubic-stabilized ZrO_2. Computer simulations of radiation damage events and damage evolution. Atomic volume swelling and radiation-induced amorphization. Application of radiation resistant oxides as matrix phases in composite materials.

168. STRUCTURAL CERAMICS: INTERFACIAL EFFECTS AND VERY HIGH TEMPERATURE MECHANICAL BEHAVIOR
T. E. Mitchell, S. P. Chen, F. Chu, A. Malloy, K. J. McClellan, J. J. Petrovic, A. F. Voter
(505) 667-0938 01-5 $643,000

Mechanical behavior of advanced structural ceramic materials: (1) Deformation and fracture studies of single crystals of oxide and non-oxide ceramics at very high temperatures. (2) Fundamental investigations of the nature and properties of interfaces important to structural ceramic composite systems. Complex oxides, silicon-based ceramics, and disilicides. Emphasis on the mechanical behavior of structural ceramics, including composites, at very high temperatures. Fundamental nature of interfaces and their role in determining mechanical behavior. Deformation behavior of single crystals of Si_3N_4,$MoSi_2$, and YAG are extended to perovskites such as $LaAlO_3$, spinels such as Mg_2CRO_4, and other complex oxides and silicides. Modeling on fracture plasticity effects and atomistic simulations of defects such as dislocations.

169. ION ENHANCED SYNTHESIS OF MATERIALS
M. Nastasi, M. Hawley, C. Maggiore, K. Walter
(505) 667-7007 01-5 $267,000

Fundamental understanding of how energetic ions influence and affect the syntheses and properties of materials. Enhanced electron emission that has been observed from diamond and diamond coated materials. Properties of materials synthesized through a plasma based ion beam processing. Relations to the plasma physics and plasma chemistry of the processing environment. This program participates in the focus project on Surface

Hardness of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

170. HIGHLY ADHERENT AND CONFORMAL HARD COATINGS FOR THE AUTOMOTIVE INDUSTRY

M. Nastasi, M. Trkula, M. Tuszewski, K. C. Walter
(505) 667-7007 01-5 $309,000

Fundamental understanding of plasma based ion processing, with energetic (hundreds of eV to many tens of keV) metallic and metalloid ions derived from high vapor pressure organometallic precursor, to produce highly adherent and conformal hard coatings for lightweight Al and Mg automotive components and automotive steel forming dies through: (1) nonequilibrium thermodynamic capabilities of plasma- and ion-solid interactions to develop new and novel materials for surface modification applications; (2) a basic understanding of the properties, stability, and deformation mechanics of plasma and ion modified materials; (3) new and novel plasma-based surface modification approaches that will provide a scientific test bed to study coating/substrate interfaces; and (4) hard coating synthesis approach that is scaleable, non-line of sight process capable of providing coatings that are conformal, relatively environmentally benign, and economical to implement.

171. METASTABLE PHASES AND MICROSTRUCTURES

R. B. Schwarz
(505) 667-8454 01-5 $220,000

Fundamental research on the theory, synthesis, microstructures, and properties of materials with metastable phases: (a) the synthesis of bulk amorphous alloys by fluxing techniques, (b) the synthesis of amorphous and nanocrystalline powders by mechanical alloying, (c) the study of phase equilibria and transformation kinetics in solid-state transformations, and (d) the application of metastable structures to improve material properties such as mechanical strength, magnetic behavior, catalysis, and superconductivity. Experimental techniques include room and high temperature X-ray diffraction, scanning and transmission electron microscopy, differential scanning calorimetry, and elastic moduli measured by resonant ultrasound spectroscopy. This program participates in the focus project on Hard Magnets of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

172. MECHANICAL PROPERTIES

M. G. Stout, U. F. Kocks
(505) 667-4665 01-5 $380,000

Response of metals to multiaxial loading and large strains, yield surfaces, multiaxial stress-strain relationships, stress path changes, Bauschinger effects. Characteristics of mechanisms controlling the large strain deformation of aluminum, nickel, iron, copper, brass, tantalum, zirconium and titanium. Sub-structural and textural evolution with strain, strain state, and strain rate. Predictions of texture evolution using crystal plasticity and strain-rate sensitivity. Kinetics of plastic flow at room and elevated temperatures. Phenomenology and mechanisms of dynamic and static recrystallization. This program participates in the focus project on Metal Forming of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

Solid State Physics - 02 -

173. CONDENSED MATTER RESEARCH WITH THE LANSCE FACILITY

J. A. Roberts
(505) 667-6069 02-1 $1,364,000

Research in condensed-matter science using the pulsed spallation neutron source, the Manuel Lujan Jr. Neutron Scattering Center, 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 vibrational spectra of organometallics; atomic arrangements of high-temperature superconductors, actinides, and metal hydrides; crystallography at high pressures; texture and preferred orientation in metallurgical and geological samples; the structure of magnetic multilayers; and residual and applied stress in engineering materials. 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, structural biology, and support science-based stockpile stewardship.

174. INTEGRATED MODELING OF NOVEL MATERIALS
S. A. Trugman, A. R. Bishop, A. F. Voter
(505) 665-1167 02-3 $474,000

This is a core program in condensed matter and materials theory aimed at extending the theory base available for modeling 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 is 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 effects of coupled spin, charge, and lattice degrees of freedom in classes of strongly correlated materials, and the development of interatomic potentials for directionally bonded materials.

175. 100 TESLA MAGNET PROJECT
L. J. Campbell, J. R. Sims
(505) 667-1482 02-4 $454,000

Design, construction, and utilization of the world's first nondestructive 100 tesla magnet user facility for materials research. This project benefits from collaboration with the National High Magnetic Field Laboratory through the shared use of power supplies, design capability, and research infrastructure. In addition to being nondestructive the magnet will have a pulse several thousand times longer than existing 100 tesla magnets and a bore size sufficiently large to accommodate milli-Kelvin refrigerators and diamond anvil cells. As a result, transport, magnetization, and optics experiments will be possible with alloys, semiconductors, organics, highly correlated electron systems, and other materials in new regions of thermodynamic phase space that, in many instances, probe quantum limits.

176. PHOTOELECTRON SPECTROSCOPY OF TRANSURANICSUTILIZING A TUNABLE UV LABORATORY LIGHT SOURCE
A. J. Arko, J. J. Joyce, P. Riseborough
(505) 665-0758 02-5 $400,000

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

177. THERMAL PHYSICS AND OSCILLATORY THERMODYNAMICS
G. W. Swift, R. E. Ecke
(505) 665-0640 02-5 $620,000

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

178. HIGH TEMPERATURE SUPERCONDUCTIVITY AND CORRELATED ELECTRON MATERIALS
J. D. Thompson, P. C. Hammel, R. H. Heffner, J. L. Sarrao
(505) 667-6416 02-5 $718,000

Effort focuses on developing a fundamental understanding of correlated electron materials by investigating the interplay among structural, magnetic and electronic properties of high-T_c and heavy fermion compounds in addition to other related narrow-band materials exhibiting valence and spin fluctuations, unconventional magnetism and superconductivity. A broad range of experimental techniques is used in these studies, including resistivity, magnetic susceptibility, specific heat, nuclear magnetic resonance, neutron diffraction and scattering, muon spin rotation, X-ray absorption fine structure, ultrasound, thermal expansion, Mossbauer spectroscopy, chemical analysis, and new materials synthesis. Many of the measurements are made at extremes of very high pressures, high magnetic fields, and very low temperatures. The approach to understanding electronic correlations in f-electron systems and applying this knowledge to the more complicated and technologically important d-electron materials provides a broad perspective on the physics of these materials.

Materials Chemistry - 03 -

179. LOW-DIMENSIONAL MIXED-VALENCE SOLIDS

B. I. Swanson, A. R. Bishop
(505) 667-5814 03-2 $267,000

This is an theoretical and experimental effort to characterize and model an extensive class of low-dimensional mixed-valence solids as they are tuned, with pressure and chemistry, from a charge-density-wave ground state towards valence delocalized sates, including spin-density-wave and spin-peierls. The systems of interest are comprised of alternating transition metal complexes and bridging groups that form linear chains and anisotropic 2- and 3-dimensional structures, with strong electron-electron and electron-phonon coupling down the chain axis. The ground and local gap states (polarons, bipolarons, excitons, biexcitons kinks, and multiphonon bound states) are characterized using structural, spectroscopic, ultra fine-resolution, transport and magnetic measurements and this information is correlated with theoretical predictions. The theoretical approach 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, including novel nonlinear and nonadiabatic features.

Facility Operations - 04 -

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

180. LUJAN CENTER OPERATIONS SUPPORT AND USER SUPPORT

J. Roberts
(505) 667-3629 04-1 $6,393,000

Neutron beams for condensed matter research at Lujan Center 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 LANSCE linac and its time-structure is tailored by a Proton Storage Ring (PSR) whose operation is supported by Defense Programs and the Office of Basic Energy Sciences. Most of the neutrons produced by proton spallation in the Lujan Center tungsten target have too high an energy to be useful for condensed matter research. To produce neutron beams of suitable energies, six moderators-four using chilled water and two using liquid hydrogen - surround the target assembly. The intense neutron beams produced by the Lujan Center target-moderator assembly provides higher instantaneous data rates than have ever been experienced before at a similar installation. To facilitate the acquisition of neutron scattering data at such an intense source, a new generation of ultra-fast, computer-based modules has been developed using the international standard FASTBUS framework. Suitable neutron scattering spectrometers make optimum use of the source characteristics provided by the PSR and the advanced target-moderator system. The spectrometers at the Lujan Center are used by researchers from government laboratories, academic, and industry. Such a national user program requires the Lujan Center support personnel to assist in the operation of spectrometers and to familiarize users with the safe operation of the facility. A scientific coordination and liaison office has been established with the responsibility for dissemination of information about the Lujan Center and coordination of the user program.

NATIONAL RENEWABLE ENERGY LABORATORY

1617 Cole Boulevard
Golden, CO 80401-3393

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

Metallurgy and Ceramics - 01 -

181. STRUCTURALLY TOLERANT ELECTRONIC OXIDES

D. Ginley, T. Ciszek, P. Parilla, J. Perkins, C. Wolverton
(303) 384-6573 01-1 $330,000

Structurally tolerant metal oxides serve as transparent conductors (SnO_2,In_2O_3) in thin film photovoltaics and flat panel displays, as electrochromic layers (WO_3) in windows and displays, and as electrodes in high energy density rechargeable Li batteries (V_2O_5 and $LiCO_2$). Oxygen off-stoichiometry and the introduction of interstitial cations. Structural tolerance to these huge defect or doping levels without structural deterioration. Relationship between the structural, electronic and optical properties. Develop a predictive model of the interplay between structure/doping, and the electronic/optical properties. New and improved oxides for important energy-related technologies. Li intercalation properties of films and single crystals of the first row transition metal oxides, in particular, LiV_2O_5 and LiC_oO_2.

182. GROWTH AND PROPERTIES OF NOVEL ORDERED II-VI AND III-V SEMICONDUCTOR ALLOYS

A. Mascarenhas, J. Olson, A. Zunger
(303) 384-6608 01-1 $679,000

This project combines experimentals with theoretical efforts aimed at understanding spontaneous long-range order in isovalent III-V/III-V and semiconductor alloys. It includes: (i) MOCVD and MBE growth of III-V alloys such as GaP/InP, AlP/GaP, AlP/InP, AlAs/InAs, and GaAs/GaP, (ii) Raman, modulation reflectance photoluminescence, spectroscopic ellipsometry and reflectance difference spectroscopy studies of ordering in the above systems, and (iii) first-principles theoretical studies of surface-induced, epitaxially-induced and bulk ordering in various alloys, as well as prediction of optical consequences of ordering (polarization anisotropy, band gap narrowing, crystal field splitting, electric fields, band offsets, NMR gradients). This program participates in the focus project on Photovoltaics of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

183. COMPUTER-AIDED PREDICTIONS OF ENERGETICS AND THERMODYNAMICS IN LIGHT-METAL AUTOMOTIVE ALLOYS

C. Wolverton, A. Zunger
(303) 384-6652 01-5 $127,000

Predictions of energetic and thermodynamic properties of light aluminum-based automotive alloys, particularly as they pertain to issues of stability, metastability, structural properties, and states of order. Clarification of the energetics and thermodynamics of these alloys, thereby leading to a more detailed understanding of processes involved in quenching experiments, precipitation kinetics, and ultimately microstructure and processing of these automotive alloys. Properties investigated by a combination of first-principles quantum and statistical mechanical calculations, affording the opportunity of stable and metastable structures, ordered and disordered alloys, and bulk and non-bulk geometries, both at zero and finite temperatures.

Solid State Physics - 02 -

184. COMPOSITION MODULATION IN SEMICONDUCTOR ALLOYS

A. Mascarenhas, E. Jones (SNL/NM), J. Reno (SNL/NM), A. Zunger
(303) 384-6608 02-2 $328,000

This is a joint project between NREL and Sandia National Laboratories involving the study of spontaneous composition modulation in III-V semiconductor alloys. The main efforts in this program are: (1) MBE growth of III-V ternary alloys and short period superlattices such as InAs/AlAs, InAs/GaAs, InP/GaP, which exhibit composition modulation, (2) Electron microscopy, Electron Diffraction, X-ray, and Atomic force microscopy studies of spontaneously compositionally modulated structures (3) Polarized Photoluminescence, Ellipsometry, Excitation Spectroscopy, Differential Absorption, Modulated Reflectance, Time resolved Photoluminescence, and Magnetoluminescence studies on spontaneously composition modulated structures, and (4) Theoretical studies on the electronic properties of compositionally modulated alloys; including large-supercell pseudopotential calculations, exploring the way that the composition modulation wavelength, amplitude and direction affects the material properties of otherwise random GaInAs, AlInAs and GaInP alloys.

185. SEMICONDUCTOR THEORY
A. Zunger
(303) 384-6672 02-3 $155,000

First-principles band structure, total energy, and statistical mechanical methods are used to predict electronic and structural properties of energy-related semiconductor superlattices, surfaces, alloys and nanostructures, emphasizing chemical trends and properties of new, energy-related materials. Current work includes (1) prediction of optical and dielectric properties of semiconductor quantum dots, wires, and films including configuration interactions (Cdse, GaAs, InP); (2) first-principles prediction of alloy thermodynamic quantities (e.g., phase-diagrams) for bulk semiconductors and metallic alloys, e.g., CuAu, CuAg, NiAu, AgAu, PdV, CuPd; (4) calculation of electronic properties of novel nitride alloys; and; (5) prediction of properties of unusual ternary materials, e.g., ordered vacancy compounds. Theoretical tools include (a) the total energy non-local pseudopotential method and full-potential linearized augmented plane wave (LAPW) method, (b) the cluster variation approach to the Ising program, applied to binary and pseudobinary phase diagrams, and (c) Monte-Carlo and simulated-annealing calculations of Ising models derived from first-principles.

OAK RIDGE INSTITUTE FOR SCIENCE AND EDUCATION
Oak Ridge, TN 37831

R. Wiesehuegel - (423) 576-3383
Fax: (423) 576-0202

Metallurgy and Ceramics - 01 -

186. SHARED RESEARCH EQUIPMENT PROGRAM
N. D. Evans, E. A. Kenik
(423) 576-4427 01-1 $267,000

The SHaRE Program fosters collaborative research between staff members in the Metals & Ceramics Division at the Oak Ridge National Laboratory (ORNL) and research staff from university, industry, or other government laboratories. While the majority of projects utilize the SHaRE User Facility at ORNL, other instrumentation within the M&C Division may be made available to external investigators. The program (1) reimburses travel and living expenses of some university personnel while at ORNL performing research. Participants from industry or other government laboratories assume their own travel and living expenses; (2) administers faculty fellowships to permit concentrated materials science research requiring the SHaRE User Facility's microanalytical facilities; and (3) provides one ORISE staff member, stationed at ORNL, who collaborates in some SHaRE research projects, assists in the administration of the of the program, instructs external participants in the operation of SHaRE facility instrumentation, and develops improved experimental equipment and techniques at ORNL which are used within the facility. Detailed descriptions of both the program and facility instrumentation can be found at URL http://www.ms.ornl.gov/share.

187. OAK RIDGE SYNCHROTRON ORGANIZATION FOR ADVANCED RESEARCH
G. Ice, J. Bai
(423) 574-2744 01-1 $108,000

A high performance X-ray beamline optimized for anomalous X-ray diffraction is made available to users from university, industrial and government laboratories. The beamline is operated jointly by the Oak Ridge National Laboratory and by the University of Illinois at Champaign/Urbana, and is located at the National Synchrotron Light Source at the Brookhaven National Laboratory. Interested scientists are invited to join in collaborative research in materials science of importance to DOE programs. More than forty scientists annually participate in experiments at this facility. The beamline provides focused X-radiation spanning the energy spectrum from 3 to 40 keV with an energy resolution $E/E \sim 2 \times 10^{-4}$. One Oak Ridge Institute for Science and Education staff member is stationed at the NSLS to interface with the users and to assist in their experiments. The beamline can be optimized for a wide range of experiments: anomalous X-ray scattering; crystallography on small samples; structure of liquid and solid amorphous materials; diffuse X-ray scattering from crystalline defects, short-range order and atomic displacements; interface studies; inelastic X-ray scattering, resonant magnetic X-ray scattering; and multiple wavelength X-ray holography. Unique X-ray instrumentation includes a dynamically-bent focusing X-ray crystal monochromator, a graphite double-focusing diffracted beam spectrometer, a split ring six circle diffractometer, and a variety of high temperature and cryogenic sample chambers with hemispherical Be domes.

OAK RIDGE NATIONAL LABORATORY

P. O. Box 2008
Oak Ridge, TN 37830

J. Ball - (423) 574-4750
Fax: (423) 574-0323

Metallurgy and Ceramics - 01 -

L. L. Horton - (423) 574-5081
Fax: (423) 574-7659

188. MICROSCOPY AND MICROANALYSIS

K. B. Alexander, J. Bentley, E. A. Kenik, M. K. Miller, K. F. Russell
(423) 574-0631 01-1 $1,795,000

Development and application of analytical electron microscopy (AEM), atom-probe field-ion microscopy (APFIM), and mechanical properties microprobes (MPM) to determine the microstructure, microchemistry and mechanical properties of materials at high spatial resolution. Operation of SHARE User facilities and collaborative research with ORNL and external users. Equilibrium and radiation-induced segregation at grain boundaries and interfaces by APFIM/AEM, correlation of grain boundary structure and segregation. Applications of advanced energy dispersive spectroscopy (EDS), electron energy loss spectroscopy (EELS), energy-filtered imaging and spectrum imaging. Radial distribution function (RDFs) by extended energy loss fine structure (EXELFS) and electron diffraction, site occupancies by Atom Location by Channeling Enhanced Microanalysis (ALCHEMI), and multivariate statistical analysis of AEM data. High-resolution scanning electron microscopy and automated electron back-scattered pattern (EBSP) texture mapping. APFIM characterization of intermetallics, phase transformations, Ni-based superalloys, bulk metallic glasses, and irradiated pressure vessel steels. AEM of structural ceramics, oxide scales, and intermetallics. MPM of thin films and electronic materials.

189. THEORETICAL STUDIES OF METALS AND ALLOYS

W. H. Butler, C. L. Fu, G. S. Painter, G. M. Stocks
(423) 574-4845 01-1 $750,000

Use of density functional theory and other techniques to calculate the properties of materials. Development of new techniques for calculating properties of materials. Use of KKR-CPA to calculate such properties of alloys as phase diagrams, thermodynamic properties, magnetic properties, lattice constants, short-range order parameters, electrical and thermal resistivities. Use of high-speed band theory (FLAPW, pseudopotential, LMTO, LKKR) to calculate total energies of metals and intermetallic compounds. Calculation of the elastic constants, and the energetics of planar and point defects of metals and intermetallic alloys, and the use of these quantities to understand their mechanical properties. Theory of electronic, magnetic, transport, magnetotransport, and tunneling properties of layered materials. 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 trace element effects on metallic cohesion. Use of tight-binding approach to study grain boundary and non-commensurate interface structures.

190. ATOMISTIC MECHANISMS IN INTERFACE SCIENCE-DIRECT IMAGING AND THEORETICAL MODELING

S. J. Pennycook, M. F. Chisholm, D. E. Jesson
(423) 574-5504 01-1 $420,000

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

191. THEORY AND DESIGN OF MONOLITHIC AND DUAL-PHASE ALLOYS BASED ON LAVES PHASE
C. T. Liu, C. L. Fu, J. A. Horton, M. H. Yoo
(423) 574-4459 01-2 $100,000

Establishment of scientific principles for enhancing low-temperature mechanical properties. First-principles calculations of electronic structure, atomic bonding characteristics, phase stability, elastic properties, deformation modes, and cleavage strength of Cr_2X-based laves alloys (X is a refractory metal element, including Nb, Zr, and Ta). Studies of point defect structure in stoichiometric and off-stoichiometric alloys. Processing of two-phase alloys containing Cr-rich solid solution and Cr_2X phases with controlled impurities and microstructures using both conventional and innovative techniques. Control of eutectic reactions in the alloys, and study of kinetics of Cr_2X precipitation in Cr-rich solid solution by TEM and SEM. Understanding and improvement of the ductility and toughness of the Cr-rich solid solution by control of impurities and microalloying additions. Investigation of interfacial structure and properties of two-phase interfaces and their role in initiation of deformation modes such as slip and twinning by a synchroshear process. Studies of interfacial structures and dislocation-particle interaction at Cr/Cr_2X interfaces. Studies of mechanical properties of two-phase Cr-Cr_2X alloys by tensile and bend tests at ambient and elevated temperatures, and establishment of microstructure-property correlations for alloy design of the two-phase alloys for high-temperature structural use. Joint research with LANL.

192. DOMAIN STRUCTURE AND DYNAMICS IN EPITAXIAL FERROELECTRICS
R. McKee, F. Walker
(423) 574-5144 01-3 $120,000

The research is examining static and dynamic structure of ferroelectric oxides through the perspective of 2-dimensionality and epitaxial constraint. An overriding difficulty in trying to develop a unifying understanding of ferroelectrics is that the microstructure of domain ordering cannot be predicted or even systematically manipulated. Molecular beam epitaxy methods, along with new insights on how to create expitaxial ferroelectrics, are being used to study domain microstructure in ferroelectric oxides. The length scales governing the thermodynamic stability of a ferroelectric phase are being studied using thin-film structures that uniquely permit the depolarization coupling to microstructure to be characterized. Collaborative research with the University of Illinois.

193. RADIATION EFFECTS
L. K. Mansur, S. W. Cook, K. Farrell, E. H. Lee, R. E. Stoller
(423) 574-4797 01-4 $1,321,000

Theoretical and experimental research on defects and microstructures produced by neutron irradiation, by ion beam treatment and by related processes. Principles for design of improved materials. Neutron damage in metals and alloys irradiated in HFIR and other reactors. Evaluation of spallation neutron radiation damage and high energy proton damage, in connection with an initiative to develop a spallation neutron source. Effect of alloying additions; effect of type of irradiation, energy spectrum, and damage rate; radiation-induced embrittlement, creep and swelling; phase stability under irradiation; relationships between ion and neutron damage; effect of helium and other impurities on microstructure and microcomposition; theory of microstructural evolution based on defect reactions. Studies using multiple simultaneous ion beams. Ion beam modification of surface mechanical and physical properties of metallic, polymeric and ceramic materials; new materials by ion beam processing.

194. MICROSTRUCTURAL DESIGN OF STRUCTURAL CERAMICS
P. F. Becher, C.-H. Hsueh, E. Y. Sun
(423) 574-5157 01-5 $974,000

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 and composites with companion studies in ceramic processing to control densification and resultant microstructure and composition in such toughened systems. These micro- and (macro-) scopic characteristics are directly related to phenomena that are controlled during powder synthesis, powder processing, and densification. These are directly coupled with studies of the role of microstructure, interfacial characteristics, composition, and defects in the mechanical behavior of ceramics and theoretical modeling of toughening-strengthening and creep mechanisms. A primary consideration of these studies is to provide the fundamental basis for the design and fabrication of advanced ceramics and ceramic composites for use over a wide range of temperatures.

195. FUNDAMENTALS OF WELDING AND JOINING
S. A. David, J. M. Vitek, T. Zacharia
(423) 574-4804 01-5 $709,000

Correlation between solidification parameters and weld microstructure; formation, distribution, and stability of microphases and inclusions; microstructure of laser-produced welds; single crystal welds; modeling of microstructure during hot cracking; theoretical models for arc plasma and weld pool interactions; modeling of transport and solidification phenomena in welds; structure-property correlations and modeling of residual stresses; austenitic stainless steels, low alloy steels, and aluminum alloys; electron beam welding; and university and industry collaborations. Processing science; computer simulation of deformation processes; modeling of microstructural evolution and correlation between microstructure and processing conditions; phenomenology and mechanisms of dynamic and static recrystallization; mechanisms controlling the large strain deformation of multi-phase materials; prediction of textural evolution and consequent material anisotropy using crystal plasticity; prediction of intergranular stresses due to inhomogeneous deformations of grains; development of novel micromechanics theories; extending the theoretical base for novel structural carbon and glass fiber polymer composites.

196. ACOUSTIC HARMONIC GENERATION BY MICROSTRUCTURES
S. A. David, O. Buck, W. A. Simpson, Jr., B. R. Thompson, J. M. Vitek, X-G. Zhang
(423) 574-4804 01-5 $249,000

Ultrasonic harmonic generation due to microstructures in materials is studied using a combination of nonlinear acoustic techniques and first-principles calculations. They study is focused in copper-aluminum alloys, and attempts to identify and separate the effects due to various types of microstructures, including solid solution effects, effects due to precipitates, voids, and dislocations. Second (and higher) harmonic responses of the alloys with different compositions and annealing histories will be measured and compared. Theoretical analysis using first-principles electronic structure techniques will help identify possible mechanisms for enhanced harmonic generation in these samples. This research is a collaboration with Ames National Laboratory.

197. THE NON-DESTRUCTIVE EVALUATION OF MATERIALS USING POSITRON SPECTROSCOPY
L. D. Hulett, Jr., G. M. Stocks, P. F. Tortorelli, M. Yoo
(423) 574-8955 01-5 $232,000

Positron spectroscopy is being used as a non-destructive method for characterizing the microstructures in:
(1) Protective oxide films on iron and nickel aluminides. Distributions of defects are being measured as a function of depth into the films, with emphasis on the interface structure. (2) A ternary amorphous alloy, $Ni_40Pd_40P_20$, from Los Alamos National Laboratory. This work will be completed in FY 1997. (3) Characterization of "ideal" microstructures (solid solution effects and voids) in copper-aluminum alloys in coordination with the "Acoustic Harmonic Generation by Microstructures" DMS program at ORNL and Ames Laboratory. This effort will allow evaluation of positron characterization of structures that are also being characterized by traditional methodologies. Research includes collaboratory with Brookhaven National Laboratory, and the Electrotechnical Laboratory, Tsukuba, Japan.

198. HIGH TEMPERATURE ALLOY DESIGN
C. T. Liu, E. P. George, J. A. Horton, C. G. McKamey, J. H. Schneibel, M. H. Yoo
(423) 574-4459 01-5 $1,149,000

Formulation of scientific principles and design of ordered intermetallic alloys based on Ni_3Al, Ni_3Si, FeAl, Fe_3Al, NiAl, FeCo, $Nd_2Fe_{14}B$, and other aluminides (e.g., TiAl) and silicides. 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 structures, solid-solution hardening, mechanistic modeling of anomalous temperature dependence of yield stress, impact resistance and crack growth, and deformation and fracture behavior of aluminides and silicides in controlled environments at ambient and elevated temperatures. Study of environmental embrittlement in intermetallic alloys and establishment of an atomic-scale understanding of this phenomenon. 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 and silicide materials prepared by conventional methods and innovative processing techniques. Establishment of correlations between mechanical properties, microstructural features, and defect structures in aluminides. Study of processing parameters on reaction kinetics and microstructural evolution of aluminides and silicides processed by reaction synthesis (combustion synthesis). This program participates in the focus projects on Design and Synthesis of Ultra High-Temperature Intermetallics, Hard Magnets and Mechanically Reliable Surface Oxides for High-Temperature Corrosion Resistance of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

199. WELDING SCIENCE FOR THE NEW GENERATION VEHICLES
M. L. Santella, S. A. David
(423) 574-4805 01-5 $317,000

An important element of the design strategy for new generation vehicles is the greater use of high strength low alloy steels to reduce weight. One of the keys to achieving this objective is the development of the science-base for the welding technologies used in the construction of automobiles. Key issues include improvements in the overall reliability and reproducibility of weld quality and weld properties. To support these goals, this research aims to develop a method for specifying welding process variables that will optimize structural integrity and reliability by developing a predictive model based on the relationship of weld properties to weld microstructures.

Solid State Physics - 02 -

J. B. Roberto - (423) 574-6151
Fax: (423) 574-4143

200. STRUCTURES OF ANISOTROPIC COLLOIDAL MATERIALS
J. B. Hayter, W. A. Hamilton
(423) 574-5239 02-1 $378,000

Small-angle neutron scattering and neutron reflectometry studies of colloidal systems. Objectives of this research are to understand the role of anisotropies imposed by geometry, shearing flow, or external fields on the structure and dynamics of liquid-phase colloidal dispersions. Major goals are to determine how anisotropic features in such systems are preserved or modified in processing to form nanoscale materials and how tuning of this behavior may be directed toward the control of the properties of final structures. In collaboration with L. Magid (University of Tennessee).

201. INSTRUMENTATION FOR NEUTRON SCATTERING
H. Mook
(423) 574-5234 02-1 $397,000

A joint effort between ORNL, the ISIS Spallation Neutron Source in England, and AT&T Bell Labs to develop advanced time-of-flight instrumentation for neutron scattering.

202. INTERATOMIC INTERACTIONS IN CONDENSED SYSTEMS
H. A. Mook, B. C. Chakoumakos, P. Dai, J. Fernandez-Baca, S. Nagler, M. Yethiraj
(423) 574-5234 02-1 $697,000

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, phase transitions, and the vortex lattice in high-temperature superconductors. New research directions will concentrate on novel materials and their properties under extreme environments of high pressures, high temperatures, or ultralow temperatures.

203. STRUCTURE AND DYNAMICS OF ENERGY-RELATED MATERIALS
H. A. Mook, S. Spooner, G. D. Wignall, M. Yethiraj
(423) 574-5234 02-1 $976,000

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 polymers, polymer blends and block copolymers, aqueous colloids (e.g., micelles, microemulsions), metal alloys, biological systems, phase transitions in polymer solutions and supercritical fluids. Residual stress mapping in welds and composite materials.

204. PROPERTIES OF ADVANCED CERAMICS
J. B. Bates, N. J. Dudney, D. C. Lubben
(423) 574-6280 02-2 $420,000

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

205. MATERIALS FOR HIGH-POWER RECHARGEABLE SOLID STATE LITHIUM BATTERIES
J. B. Bates, N. J. Dudney, D. C. Lubben
(423) 574-6280 02-2 $409,000

Synthesis and processing of thin and thick films of lithium intercalation cathode materials. Present emphasis on the spinel phase of lithium manganese oxide, $LiMn_2O_4$. Methods for thin-film deposition include rf magnetron sputtering and electron beam evaporation. Single-phase and composite thick films are fabricated by tape casting methods. Films are characterized by X-ray diffraction, infrared and optical spectroscopy, Rutherford backscattering, electron microscopy, and impedance spectroscopy. Cathodes are also investigated in solid state lithium cells. Constant current cycling of the cells and in situ X-ray diffraction are used to evaluate further the electrochemical properties of the cathode films and the changes in structure with lithium intercalation and deintercalation.

206. SYNTHESIS AND PROPERTIES OF NOVEL MATERIALS
L. A. Boatner, D. G. Mandrus, J. O. Ramey, B. C. Sales
(423) 574-5492 02-2 $912,000

Synthesis and characterization of advanced materials including single crystal growth and the development of new crystal growth techniques; development of new materials using enriched stable isotopes; investigations of the physical, chemical, and thermal properties of novel materials using the techniques of thermal analysis, X-ray diffraction, Mossbauer spectroscopy, magnetic susceptibility, electrical transport, ion implantation and RBS/ion channeling, optical absorption, high-performance liquid chromatography, EPR, atomic force microscopy, and X-ray or neutron scattering; application of materials science techniques to basic research problems; preparation and characterization of high T_c superconducting oxides; synthesis and structural characterization of phosphate glasses; development and characterization of advanced ceramics and textured materials; solid state epitaxial regrowth; growth of perovskite-structure oxides, in bulk and thin-film forms; high-temperature materials (MgO, CaO, $LaPO_4$), refractory metal single crystals (Nb, Ta, V), fast-ion conductors, thermoelectric materials, magnetic materials, stainless steels, rapid solidification and solidification microstructures; new scintillator, thermophosphor and photonic materials; new fiber; and detector materials, "smart" surfaces and materials.

207. PHYSICAL PROPERTIES OF SUPERCONDUCTORS
D. K. Christen, R. Feenstra, H. R. Kerchner, J. R. Thompson
(423) 574-6269 02-2 $462,000

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

208. X-RAY RESEARCH USING SYNCHROTRON RADIATION
G. E. Ice, E. D. Specht
(423) 574-2744 02-2 $379,000

Research focuses on the use of synchrotron radiation as a probe for the study of metal alloys, ceramics, and interfaces, emphasizing the ability to select a particular X-ray energy from the synchrotron radiation spectrum to highlight atomic arrangements of specific elements. Thus, the atomic arrangements among the various elements can be unraveled and related to the materials' physical and chemical properties. Microfocused X-ray beams will extend applications to submicron resolution. The task includes operation of an X-ray beamline on the National Synchrotron Light Source at Brookhaven National Laboratory. Staff are also involved in the design, construction, and operation of two X-ray beamlines on the Advanced Photon Source. Important materials' problems under study include: (1) effects of short-range order among atoms on mechanical, chemical and magnetic behavior and on radiation swelling; (2) effects of atomic displacements, caused by bonding and size difference, on energetics of phase stability and materials properties; (3) effects of epitaxy and film thickness on phase transitions, and (4) role of atomic-scale structure and chemistry of interfaces in controlling heteroepitaxy.

209. SEMICONDUCTOR PHYSICS, THIN FILMS, AND PHOTOVOLTAIC MATERIALS
D. H. Lowndes, G. Eres, D. B. Geohegan,
G. E. Jellison, D. P. Norton
(423) 574-6306 02-2 $867,000

Fabrication of superconducting, semiconducting, and optical thin films by pulsed-laser ablation and molecular jet CVD energetic-beam growth methods, growth and doping of elemental and compound semiconductors for thin-film photovoltaics; in-plane aligned substrates for high-Jc superconducting films; laterally selective film growth by pulsed-jet CVD and e-beam writing; epitaxial growth of modulated layered structures and superlattices; time-resolved measurements of pulsed-laser-generated plasmas using optical emission, absorption, ion probe, and gated photographic methods; time-resolved and scanning ellipsometric measurements; studies of semiconductor film-growth reactions and growth and defect formation mechanisms; pulsed-laser bonding of metals to ceramics; thermal and laser annealing of lattice damage in semiconductors; fabrication of solar cells by laser, and thin-film techniques; effects of point defects and impurities on electrical and optical properties of elemental and compound semiconductors; current-voltage and resistance-temperature measurements of superconducting transitions and dissipation. Scanning tunneling microscopy, transmission electron microscopy, X-ray scattering, secondary ion mass spectrometry, and Rutherford ion backscattering measurements; photon- and electron beam lithography; dopant concentration profiles, deep-level transient spectroscopy, and solar cell electrical characteristics; and spectral response absolute quantum efficiency measurements.

210. SYNTHESIS OF NONEQUILIBRIUM MATERIALS AND STRUCTURES USING LASER-MBE
D. H. Lowndes, G. E. Jellison, B. C. Larson,
D. P. Norton, E. D. Specht, J. Z. Tischler, Z. Zhang
(423) 574-5506 02-2 $486,000

Fundamental studies of nonequilibrium growth of thin-film materials and structures in reactive environments, using energetic pulsed-laser ablation beams and in situ, time-resolved synchrotron X-ray measurements. Use of pulsed-laser deposition, combined with the high intensity and pulsed time structure of synchrotron X-rays at the Advanced Photon Source, to separate fundamental growth steps of deposition and aggregation in order to directly probe the formation and evolution of crystalline structure, from the arrival of incident species (atoms, ions, and clusters) through crystallization. Simulations using massively parallel computers to understand kinetics of nonequilibrium growth under pulsed reactive conditions; dopant/defect complexes; and nonequilibrium materials properties. Correlation of initial and intermediate growth configurations with final film structures to understand the effect of deposition conditions on each phase of growth. Development of real-time, in situ scanning ellipsometry to monitor film and multilayer growth in reactive environments; correlation with synchrotron measurements to enable nonequilibrium growth monitoring by ellipsometry in remote locations and industrial environments. Growth of YBCO and infinite-layer high-temperature superconductors; II-VI and I-III-VI2 compound semiconductors. Reflection high-energy electron diffraction, atomic force microscopy, transmission electron microscopy, Rutherford ion backscattering, optical and electrical properties measurements.

211. SMALL-ANGLE X-RAY SCATTERING
G. D. Wignall, J. S. Lin, S. Spooner
(423) 574-5237 02-2 $164,000

Small-angle X-ray scattering (SAXS) from a wide variety of materials in the solid (e.g., polymers, metals, alloys), liquid (e.g., zirconium suspensions, surfactants, aqueous colloids), and gaseous states (e.g., polymers in supercritical fluids). SAXS is also used to study domain structures in composite materials; aggregation mechanisms in sol-gels and for time-slicing studies of phase transformations in polymer blends, block is polymers and alloys. Facilities are available to users at no charge for research published in the open literature or under contract for proprietary research.

212. THEORY OF CONDENSED MATTER
J. F. Cooke, A. G. Eguiluz, R. S. Fishman, D. Mahan,
C. Marinescu, R. F. Wood, Z. Zhang
(423) 574-5787 02-3 $883,000
Electrical and thermal transport across and along grain boundaries, lattice vibrations in metals and alloys. Atomistic studies of surfaces and interfaces including relaxation, electronic structure of metal surfaces, magnetism in transition metals and local moment systems, magnetic multilayers, neutron scattering at high energies. High-temperature superconductivity, quantum Hall effect, studies of thermoelectric and varistor-related phenomena, computer modeling of the laser ablation technique, ab initio calculations of the dynamic properties of metallic systems, nonequilibrium growth phenomena, and quantum engineering of metallic thin-film growth.

213. STRUCTURAL PROPERTIES OF MATERIALS - X-RAY DIFFRACTION
B. C. Larson, J. D. Budai, J. Z. Tischler
(423) 574-5506 02-4 $403,000

Microstructure and microstructural of defects in solids, synchrotron X-ray scattering, microbeam X-ray scattering microbeam X-ray scattering, time-resolved X-ray scattering, growth and structure of pulsed laser deposited films, inelastic X-ray scattering, ion implantation formation of nanocrystals in materials, X-ray diffuse scattering, Mossbauer scattering spectroscopy, X-ray topography, ion implantation formation of nanocrystals in materials, pulsed-laser-induced melting and crystal growth, defects associated with laser and thermal processing of pure and ion-implanted semiconductors, microstructural characterization of high-temperature superconducting films, on single-crystal and textured substrates, theory of scattering of X-rays from defects in solids.

214. ELECTRON MICROSCOPY OF MATERIALS
S. J. Pennycook, M. F. Chisholm, D. E. Jesson
(423) 574-5504 02-4 $542,000

Atomic resolution scanning transmission electron microscopy and electron energy loss spectroscopy; theory of elastic, inelastic, and diffuse scattering of electrons from crystals and defects; simulation of Z-contrast images and electron energy loss near-edge structure. Growth and relaxation phenomena in epitaxial thin films; interface structure/property relations; morphological stability; molecular beam epitaxial growth; structure of catalysis; ion implantation; segregation phenomena.

215. INVESTIGATIONS OF SUPERCONDUCTORS WITH HIGH CRITICAL TEMPERATURES
D. K. Christen, J. D. Budai, H. R. Kerchner,
D. P. Norton, S. J. Pennycook, B. C. Sales
(423) 574-6269 02-5 $439,000

Studies of superconducting materials with high transition temperatures. Synthesis, characterization, and analysis of thin films, thin-film heterostructures, new substrate materials, single crystals and melt-processed bulk materials, and high-current coated conductors and composite structures. Magnetic and electrical transport properties, microstructural characterization by electron microscopy. Collaborative research with scientists at IBM Watson Research Center, The University of Tennessee, SUNY-Buffalo, University of Houston, and other U.S. universities.

216. RADIATION SAFETY INFORMATION COMPUTATIONAL CENTER (RSICC)
B. L. Kirk, R. W. Roussin
(423) 574-6176 02-5 $71,000

This task is directed in support of basic energy sciences for application to a wide variety of radiation effects, radiation transport, shielding, and neutronics problems. It provides information and technology which contributes to the solution of problems occurring in DOE programs for materials sciences, and other basic energy sciences. In FY 1997 there were 39 individuals from 20 organizations who have registered with the Radiation Safety Information Computational Center (RSICC) and indicated they are working on DOE/BES projects. The level of RSICC activity on behalf of BES contractors is increasing. RSICC is a technical institute, serving DOE radiation research and development programs by collecting, organizing, processing, evaluating, packaging, and disseminating information related to radiation transport and safety. The scope includes physics of interaction or radiation with matter, radiation production and radiation transport, radiation detectors and measurements, engineering design techniques, shielding materials properties, computer codes useful in research and design, and shielding data compilations. In addition, RSICC participates in CSEWG activities and processes cross sections for its sponsors, gives leadership to shielding computing standards activities (ANS-6 and -10) and organizes seminar workshops as needed. RSICC is partially supported by DOE's Nuclear Energy Program, Office of Defense Programs, Office of Environmental Management, Office of Environment, Safety and Health, Office of Nonproliferation and National Security, and the Office of Fusion Energy, and by the Defense Special Weapons Agency (DSWA). By integrating developments in the various programs (fission and fusion reactors, nuclear weapons, accelerators) the latest technology is made available to all scientists and engineers doing radiation transport calculations.

217. SURFACE MODIFICATION AND CHARACTERIZATION FACILITY AND RESEARCH CENTER
D. B. Poker, S. P. Withrow
(423) 576-8827 02-5 $1,110,000

The SMAC Collaborative Research Center provides facilities for materials alteration and characterization in a UHV environment. Methods which can be used for alteration include ion implantation, ion beam mixing, and low-energy ion deposition using 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 such as low-energy electron diffraction and Auger electron spectroscopy. The facility supports research in the Ion Beam Analysis and Ion Implantation Program as well as other programs in the Solid State Division 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.

218. ION BEAM ANALYSIS AND ION IMPLANTATION

C. W. White, T. E. Haynes, O. W. Holland, R. A. Zuhr
(423) 574-6295 02-5 $711,000

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; formation of nanocrystals and quantum dots in a wide variety of substrates by 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, and characterization of superconducting thin films; fundamental studies of ion beam mixing in metal/semiconductor, metal/metal, and metal/insulator systems; applications of ion beam mixing and ion implantation to corrosion/catalysis studies, to reduction of friction and wear of metal surfaces, to changes in mechanical and optical properties of ceramics and insulators, to the formation of nonlinear optical materials, and to reduction of corrosive wear of surgical alloys; studies of ion channeling phenomena; direct ion beam deposition (IBD) of isotopically pure thin films, using decelerated, mass-analyzed ion beams.

219. SURFACE PHYSICS

D. M. Zehner, A. P. Baddorf, A. K. Swan, J. F. Wendelken
(423) 574-6291 02-5 $819,000

Studies of crystallographic and electronic structure of clean and adsorbate-covered metallic, intermetallic compound, carbide, and semiconductor surfaces; combined techniques of low-energy electron diffraction (LEED), photoelectron spectroscopy using synchrotron radiation, scanning tunneling microscopy (STM), and computer simulations for surface crystallography studies. LEED, Auger Electron Spectroscopy and X-ray photoelectron spectroscopy studies of both clean and adsorbate-covered surfaces; determination of effects of intrinsic and extrinsic surface defects on surface properties, surface and thin-film growth morphology, and surface magnetism using high-resolution LEED and STM and surface magnetic optical Kerr effect; vibronic structure of surfaces and adsorbates examined by high-resolution electron energy loss spectroscopy; examination of surface electronic and geometric structures with respect to solid state aspects of heterogeneous catalysis.

220. NATIONAL SPALLATION NEUTRON SOURCE CONCEPTUAL DESIGN

B. R. Appleton
(423) 574-4321 02-6 $7,668,000

The Spallation Neutron Source (SNS) is an accelerated-based, pulsed, spallation neutron source that will be used for the neutron scattering needs of the DOE and the scientific community. The facility will consist of an ion source, full-energy conventional linac and accumulator ring that bombards a liquid mercury target where neutrons are produced in a nuclear reaction process called spallation. The source will provide neutrons to 18 beam lines where neutron scattering instruments are located. Funding in FY 1996 and FY 1997 was used to complete the Conceptual Design Report (CDR) for SNS for the DOE/ER. A consortium of five DOE National Laboratories (ANL, LANL, BNL, LBNL, and ORNL) was formed by ORNL to establish the reference design and technical approach, and to perform the R&D leading to the CDR. On June 23-27, 1997, DOE/ER performed a full validation review of the technical feasibility, cost, schedule, management, and S&H approach of SNS. The CDR Review Committee strongly endorsed SNS and provided their recommendations to DOE. The cost and schedule information from this review will be used to request a construction line item for SNS in the FY 1999 budget.

Materials Chemistry - 03 -

M. L. Poutsma - (423) 574-5028
Fax: (423) 576-5235

221. CHEMISTRY OF ADVANCED INORGANIC MATERIALS

D. B. Beach, M. Paranthaman, C. E. Vallet
(423) 574-5024 03-1 $847,000

Synthesis of inorganic thin-film solid-state materials by the decomposition of molecular precursors. Of particular interest are epitaxial multi-element oxide films on single crystal substrates. Synthetic routes include sol-gel, metal organic decomposition (MOD) and metal organic chemical vapor deposition (MOCVD). Underlying each of these techniques is the solution chemistry of metal alkoxides, metal carboxylates, and metal coordination compounds which we study using multi-nuclear NMR, FTIR, thermal analysis, X-ray scattering, and other techniques. Classes of compounds under investigation include cuprate superconductors, buffer layers for cuprate superconductors, films for the remote monitoring of strain and temperature, and various electronic and optoelectronic ceramics. Techniques for materials characterization include atomic force microscopy (AFM), scanning tunneling microscopy (STM), Rutherford backscattering spectroscopy (RBS), X-ray diffraction (XRD), and a variety of electrical, magnetic, and optical measurement techniques.

222. THERMODYNAMICS AND KINETICS OF ENERGY-RELATED MATERIALS

E. C. Beahm
(423) 574-6851 03-2 $247,000

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

223. STRUCTURE AND DYNAMICS OF ADVANCED POLYMERIC MATERIALS AND NANOPHASE BLENDS

A. Habenschuss, B. K. Annis, J. G. Curro (SNL/NM), D. W. Noid, K. S. Schweizer, B. G. Sumpter, G. D. Wignall, B. Wunderlich
(423) 574-6018 03-2 $1,103,000

Characterization of polymers at the molecular level by scattering methods, thermal and mechanical analysis, microscopy, spectroscopy, molecular simulations, and design and prediction of polymer materials properties. Materials of interest range from bulk polymers, films, fibers, copolymers, polymer blends and composites. Varying degrees of molecular ordering are being investigated, including the crystalline, semicrystalline, mesophase (liquid-, plastic-, and condis-crystals) and amorphous states (glasses, melts). State-of-the-art computational methods such as molecular dynamics, Monte Carlo, quantum chemistry, neural networks, graph theory, and genetic algorithms are used to model polymeric structure and dynamics. Emphasis on developing a scientific basis for the molecular design of multicomponent polymer blends, where mixing occurs on molecular length scales. Our approach combines experimental characterization by scattering methods, theoretical modeling, and synthesis to predict and characterize blend structure, miscibility, phase diagrams, and thermodynamic properties.

224. NUCLEATION, GROWTH, AND TRANSPORT PHENOMENA IN HOMOGENEOUS PRECIPITATION

Z.-C. Hu, C. H. Byers
(423) 574-8782 03-2 $233,000

Fundamental laser light-scattering, X-ray scattering/diffraction, and spectroscopic studies are conducted on and a theoretical framework is developed for liquid-phase homogeneous nucleation and growth of pure component and composite monodisperse metal oxide particles. These particles are precursor materials in ultra fine processing for the production of a new generation of structural and functional ceramic materials. The program includes investigation of metal alkoxide/metal salt reactions and reactant-solvent interactions which affect the characteristics of the particles formed. Methods and instrument development (including alternative methods for chemical synthesis of metal oxide ultra fine powder and nanostructured materials, optical spectroscopic measurements, low angle-light scattering, flow through

SAXS and FTIR, colloidal, dispersion stability, HTXRD, Raman, and NMR spectroscopy mathematical analysis) are important features of this research.

PACIFIC NORTHWEST NATIONAL LABORATORY

P. O. Box 999
Richland, WA 99352

G. McVay - (509) 375-3762
Fax: (509) 375-2186

Metallurgy and Ceramics - 01 -

225. MICROSTRUCTURAL MODIFICATION IN CERAMIC PROCESSING USING INORGANIC POLYMER DISPERSANTS

G. J. Exarhos, J. Liu, W. D. Samuels, L.-Q. Wang
(509) 375-2440 01-1 $270,000

Fundamental research focused on interparticle interactions in colloidal suspensions, molecular-directed assembly of three-dimensional ceramic architectures, and synthesis of polymer-ceramic molecular composites. Modification to interfacial bonding in composites through changes in processing chemistry. Modeling studies to simulate the magnitude of these interactions and how they can be perturbed through surfactant modification, choice of solvent, and chemical alteration to particle surface sites. Characterization of molecular interactions in the evolving nanostructure by means of in situ magnetic resonance and vibrational spectroscopy measurements at all stages during processing. Evaluation of physical properties and microstructure derived from electron and atomic force microscopies to understand how processing routes alter material properties. This program participates in the focus project on Microstructural Engineering with Polymers of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

226. INTERFACIAL DYNAMICS DURING HETEROGENEOUSDEFORMATION

S. M. Bruemmer, C. H. Henager, Jr., J. S. Vetrano
(509) 376-0636 01-2 $450,000

The purpose of this research is to elucidate mechanisms controlling heterogeneous, interfacial deformation processes through a combination of high-resolution measurement and atomistic modeling techniques. Emphasis is placed on characterizing, modifying, and simulating dynamic events occurring at grain boundaries and particle-matrix interfaces. Specific interfacial processes such as dislocation emission and accommodation, boundary migration, sliding, diffusion, solute segregation, and cavitation will be isolated and evaluated. Initial research focuses on the interfacial dynamics limiting the superplastic deformation of fine-grained metallic materials. Synergistic effects of stress, strain, strain rate, and temperature on grain boundary composition, dislocation activity, and properties are being examined in controlled purity alloys. Fundamental relationships and understanding will be established to give mechanistic insight into empirical continuum equations of interfacial deformation processes. This program participates in the focus project on Metal Forming of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

227. FUNDAMENTAL STUDIES OF STRESS CORROSION AND CORROSION FATIGUE MECHANISMS

R. H. Jones, C. H. Henager Jr., E. P. Simonen, C. F. Windisch, Jr.
(509) 376-4276 01-2 $342,000

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 effects of grain boundary microchemistry on crack growth in nickel- and iron-based alloys. Differential, reversed dc potential drop analysis of stress corrosion initiation and cracking processes. Effect of surface chemistry on gas phase adsorption and aqueous corrosion using transient electrochemical analysis. This program participates in the focus project on Materials Joining of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

228. CHEMISTRY AND PHYSICS OF CERAMIC SURFACES
B. C. Bunker, S. A. Chambers, K. F. Ferris, M. A. Henderson, S. A. Joyce, L. Q. Wang
(509) 375-5969 01-3 $450,000

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

229. IRRADIATION-ASSISTED STRESS CORROSION CRACKING
S. M. Bruemmer, D. J. Edwards, E. P. Simonen, G. S. Was (Univ. of Michigan)
(509) 376-0636 01-4 $460,000

The mechanisms controlling irradiation-assisted stress corrosion cracking under neutron and charged-particle irradiation are evaluated using experiments and modeling. Research includes radiation effects on grain boundary composition, matrix and interfacial deformation processes, crack-tip phenomena, and material electrochemical behavior. Radiation-induced grain boundary segregation is measured and modeled as a function of material and irradiation parameters. Specific grain boundary compositions and matrix microstructures are simulated by thermomechanical treatments, and their influence on corrosion and stress corrosion assessed by tests in low- and high-temperature aqueous environments. Crack-tip models are developed so that radiation effects on local material microstructure, microchemistry, deformation, and electrochemistry can be assessed in relation to crack propagation mechanisms.

230. IRRADIATION EFFECTS IN CERAMICS
W. J. Weber, N. J. Hess, R. E. Williford
(509) 375-2299 01-4 $221,000

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

231. ENVIRONMENTAL DEGRADATION MECHANISMS IN LIGHTWEIGHT TRANSPORTATION ALLOYS
R. H. Jones, M. J. Danielson, J. S. Vetrano, R. E. Williford
(509) 376-4276 01-5 $234,000

Investigations of the critical environmental degradation mechanisms in lightweight automotive alloys including nonheat treatable Al sheet (Al-Mg), superplastically formed aluminum alloys and magnesium alloys. Evaluation of grain boundary microchemistry and microstructural causes for stress corrosion and other processes that could potentially inhibit these effects in Al-Mg alloys. Measurement of grain boundary segregation using Auger electron spectroscopy (AES) and analytical electron microscopy, surface and electrochemical reactions with Laser Raman, AES, X-ray photoelectron spectroscopy and a surface analytical tool-corrosion side cell, early stages of intergranular cracking using atomic force microscopy, and electrical potential drop methods to measure the crack velocity of very short cracks. Evaluation of alloys with additives that could potentially inhibit stress corrosion cracking in Al-Mg alloys.

232. DESIGN AND SYNTHESIS OF NANOSCALE ULTRACAPACITOR MATERIALS USING LYOTROPIC LIQUID CRYSTAL TEMPLATES
J. W. Virden, S. H. Elder, J. Liu, C. F. Windisch
(509) 375-6512 01-5 $250,000

This research focuses on the formation mechanisms of mesoporous ceramic oxides synthesized from surfactant nanostructural templates. Integrated experimental and modeling efforts will investigate the surfactant selection and control of surfactant interactions to promote and optimize nucleation and growth of ceramic phases into specific nanostructures. Research investigates surfactant interactions leading to surfactant self-assembly and interaction between surfactant arrays (i.e., micelle-micelle interactions) that influence pore size, wall thickness, and overall surface area. Control of pore size and wall thickness relates to sinterability of oxides and conversion to high-surface area conductive nitrides or carbides. Characterization of the evolution of the final ultracapacitor material from soluble precursor to templated oxide to final conductive mesoporous ceramic will establish structure-property relationships to optimize ultracapacitor performance.

Solid State Physics - 02 -

233. THIN FILM OPTICAL MATERIALS
G. J. Exarhos, K. F. Ferris, C. F. Windisch, Jr.
(509) 375-2440 02-2 $197,000

Integrated experimental and theoretical studies designed to understand how materials properties including residual stress, surface morphology, and phase homogeneity correlate with the attendant linear and nonlinear optical response of dielectric films deposited using both vacuum and solution-based methods. Issues addressed include phase stability, stress homogeneity, the resident microstructure which evolves during deposition, and the associated perturbation in film optical properties when subjected to variations in temperature, pressure, electric field or chemical environment. Finite element modeling approaches provide insight into structure/property relationships. Development of innovative deposition techniques and post-deposition modification routes for the mainupulation if film microstructure and chemical state in order to attain a targeted optical response. Application of AFM, Raman and fluorescence methods, ellipsometry, and electron spectroscopy for film characterization. This program supports the photovoltaics task within the DOE Center of Excellence for the Synthesis and Processing of Advanced Materials.

Materials Chemistry - 03 -

234. CERAMIC COMPOSITE SYNTHESIS UTILIZING BIOLOGICAL PROCESSES
A. A. Campbell, G. E. Fryxell, G. L. Graff, P. C. Rieke, L. Song, B. J. Tarasevich
(509) 375-2833 03-1 $471,000

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

SANDIA NATIONAL LABORATORIES-CALIFORNIA
P.0. Box 969
Livermore, CA 94551-0969

W. L. Bauer- (510) 294-2994
Fax: (510) 294-3231

Metallurgy and Ceramics - 01 -

235. SURFACE, INTERFACE, AND BULK PROPERTIES OF ADVANCED CERAMICS
K. F. McCarty, D. L. Medlin
(510) 294-2067 01-1 $404,000

The major focus of this project is the synthesis and characterization of novel, thin-film structures of ultrahard and wide-bandgap ceramics. We emphasize ion-assisted deposition, and the use of in-situ diagnostics during film growth. The project focuses on nitride ceramics, including the boron and aluminum nitride systems. We strive for a fundamental understanding and quantitative models of ion-assisted film growth, including the microscopic mechanisms controlling selective formation of, for example, (diamond-like) cubic boron nitride over the stable (graphite-like) phase. Multilayer ceramic structures will be synthesized and characterized with the goal being engineered mechanical and electronic properties. We study the microstructure, phonon structure, and electronic defect structure of the thin films using Raman spectroscopy, infrared spectroscopy, photoluminescence, and transmission electron microscopy. Mechanical-property measurements are performed to evaluate both fundamental properties and technological viability. This program participates in the focus project on Processing for Surface Hardness of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

236. DYNAMICS OF DISLOCATIONS IN THIN FILMS

R. Q. Hwang, N. C. Barelt, C. B. Carter (Univ. of Min.), D. Gibbs (BNL), J. C. Hamilton, D. M. Zehner (ORNL)
(510) 294-1570 01-2 $250,000

The objective of this program is to quantitatively understand the dynamics of dislocations in thin films. These kinetics are responsible for defining the mechanical behavior and plastic response of thin films as well as being crucial to their chemical properties. A key aspect to this problem is forging the link between the atomistic processes that are responsible for mass transport and the longer length scales related to dislocation structures and their strain fields. Our approach is to use in-situ time resolved techniques such as the scanning tunneling microscopy, glancing incidence X-ray diffraction and electron microscopy to image dislocation motion under controlled environments. This information will be coupled to theoretical work to developed useful models of these dynamics. Our current emphasis is to understand the atomistic processes that govern threading ana partial dislocation motion in fcc(111) oriented films. Such motion involves a complex combination of diffusion and incorporation of adatoms and vacancies and the influence of thin film strain. Building a fundamental understanding of dislocation dynamics is crucial to the ability to predict the time evolution of materials under mechanical, chemical and electronic forces.

237. DEFECTS AND IMPURITIES IN SOLIDS/COMPUTATIONAL MATERIALS SCIENCE/VISITING SCIENTIST PROGRAM

W. G. Wolfer, N. C. Bartelt, S. M. Foiles, J. C. Hamilton, J. R. Hoffelfinger, D. A. Hughes, R. Q. Hwang, C. L. Kelchner, D. L. Medlin, A. A.. Quong, A. K. Schmid, P. O. Tepesch
(510) 294-2307 01-2 $1,004,000

These three programs will enhance our understanding, in quantitative terms, of defects in solid materials. This understanding is to span length scales from the atomic to the microstructural, and will relate to macroscopic properties and the performance of materials in various applications. The quantitative understanding is captured both in mathematical relationships and in computational methods and tools suitable for wide application to materials science and technology. Furthermore, the methods and tools are to complement each other so that all length as well as time scales (from the period of atomic vibrations to the lifetime of an engineering component) can be joined and covered. The approach is to support both experimental and theoretical research on the same, or closely related, topics in an environment that induces communication and close collaboration between experimentalists and theoreticians. The Visiting Scientist Program facilitates collaborations with researchers at other institutions. Presently, the experimental program "Defects and Impurities in Solids" focuses on STM, AFM, and electron diffraction investigations of multi-elemental surface layers, films and coatings; on HRTEM studies of the structure of dislocation cores, grain boundaries, and interfaces; and on the dislocation cell structure in plastically deformed metals. The major activities in the "Computational Materials Science" program include the following thrusts: electronic structure methods including LDA/pseudopotential segregation and thermodynamic properties and a linear response code to compute the dynamical properties; atomistic simulation methods based on an order-N tight binding method as well as empirical potentials; statistical analysis of ordering, segregation and thermodynamic properties; and studies of kinetics based on kinetic Monte Carlo schemes and continuum evolution equations. Each development is carried out in the context of the experimental activities and/or specific applications in materials science and technology.

238. FIRST PRINCIPLES COMPUTATIONS FOR ALLOY DESIGN

M. Asta, J. D. Althoff (Univ. of CA), S. M. Foiles, J. J. Hoyt, A. A. Quong, W. G. Wolfer, D. de Fontaine
(510) 294-1355 01-3 $418,000

The goal of this program is to predict the thermodynamic properties of multicomponent crystalline and liquid alloys from first-principles calculations. Since the energy differences between stable and metastable alloy phases are typically small, realistic calculations of alloy properties must make use of the accuracy available from first-principles, electronic-structure methods. For the purpose of applying these methods to multicomponent systems and to alloy phases which possess both topological and compositional disorder, theoretical approaches are being developed in three areas. First, for multicomponent alloys we are formulating systematic approaches for decoupling chemical degrees of freedom in order to simplify energetic models, and generalized mean-field statistical-mechanical algorithms are being developed for calculating finite-temperature thermodynamic properties. Secondly, since phase transformations frequently involve a change in the underlying lattice structure, first-principles methods to treat the coupling between structural and compositional disorder in alloys are being developed. In particular, we use the results of first-principles calculations for alloy formation energies and interatomic force constants to parametrize energy models which incorporate both configurational and displacive degrees of freedom. Finally, in order to model amorphous alloy formation, and in order to be able to calculate liquidus and solidus phase boundaries, we exploit perturbation-theory treatments of solid-liquid free-energy differences combined with the above first-principles methodologies for crystalline alloys to calculate liquid-phase thermodynamic properties. The ultimate outcome of this work will be a predictive theory of alloy properties that is useful in alloy design. As an example, the computational framework will be used to search for deep eutectics in multicomponent systems, thereby guiding the development of novel amorphous metal alloys.

239. ALLOY THEORY

D. D. Johnson, M. D. Asta, F. J. Pinski (Univ. of Cinn)
(510) 294-2751 01-3 $1,355,000

A "first-principle" theory for alloys is developed in which electronic, size, charge-transfer, and magnetic effects (which are responsible for the effective interactions between the alloy constituents) play an essential role in determining the phase diagrams and the ordering tendencies in disordered alloys. Correlation functions for compositional and magnetic short-range ordering are derived from the theory and utilized to interpret experimental results from diffuse X-ray and neutron scattering experiments, and to further plan and guide such experiments. The combined theoretical and experimental efforts elucidate the underlying electronic forces for intermetallic interactions and their influence on the thermodynamics of alloys including ordering in multicomponent alloys, such as ternaries. Finally, the theory will be used to explore and discover new metal alloys, and the electronic origin for their ordering properties projects on Metals Forming and on Materials Joining of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

Solid State Physics - 02 -

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240. MATERIALS CHARACTERIZATION USING ULTRAFAST OPTICAL TECHNIQUES

R. J. Anderson
(510) 294-3258 02-2 $176,000

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

SANDIA NATIONAL LABORATORIES-NEW MEXICO

P. 0. Box 5800
Albuquerque, NM 87185

G. Samara - (505) 844-6653
Fax: (505) 844-4045

Metallurgy and Ceramics - 01 -

241. PHYSICS AND CHEMISTRY OF CERAMICS

R. A. Assink, T. Alam, T. J. Boyle, C. J. Brinker, R. K. Brow, K. Chen, A. J. Hurd, P. R. Schunk, R. W. Schwartz, D. R. Tallant
(505) 845-8629 01-2 $968,000

For glasses and sol-gel-derived ceramics, we measure and model the effects of processing on molecular structure, network topology, pore formation and behavior, network dynamics, crystallite growth and sintering. Our tools include NMR, small-angle X-ray scattering, fluorescence, neutron scattering, quasielastic light scattering, dynamic mechanical analysis, dielectric relaxation, materials modeling and imaging ellipsometry to establish structure and behavior across a wide range of spatial and temporal scales in solutions, films, and monoliths. The theme in the Physics and Chemistry of Ceramics Program has long been that of borrowing from nonceramic fields: nonequilibrium, kinetic processes that lead to fractal structures, anomalous diffusion models, and concepts from polymer physics are examples of the new viewpoints we have applied recently to solution precursors and the dynamics of glasses. Ceramics and glasses are increasingly used in demanding, high consequence situations. "Perfectly" assembled materials will never be realized, but our goal is to understand the processes that link precursors to the properties of materials. This program participates in the focus projects on Microstructural Engineering with Polymers and Materials Joining of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

242. ATOMIC LEVEL SCIENCE OF INTERFACIAL ADHESION

T. A. Michalske, A. Burns, P. J. Feibelman, J. E. Houston, R. C. Thomas
(505) 844-5829 01-2 $424,000

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.

243. WETTING AND FLOW OF LIQUID METALS AND AMORPHOUS CERAMICS AT SOLID INTERFACES

N. D. Shinn, U. Landman (Georgia Tech.), T. A. Michalske
(505) 844-5457 01-2 $275,000

The objective of this program is to provide a scientific basis to understand the nanometer-scale structure, chemistry and flow properties of liquid metals and amorphous ceramics at solid interfaces. We will develop a fundamental understanding of the wetting and flow properties of interfacial liquids that combines: (1) new atomic scale methods for measuring the wetting and flow of liquids near well characterized interfaces, (2) theoretical simulations for liquid flow and stability, and (3) macroscopic wetting, spreading, and creep measurements that can be used to relate the results of fundamental experiment and theory to practical materials response. Key to our unique approach is the ability to make detailed measurements of the wetting and flow of atomically thin, well characterized liquid metal and amorphous ceramic interfacial layers. These measurements will provide a common point that will permit interactions extending from atomic-level theory to practical wetting and flow measurements and will provide fundamental insight into the factors controlling the wetting and flow of thin liquid layers.

244. ADVANCED GROWTH TECHNIQUES AND THE SCIENCE OF EPITAXY
E. Chason, J. A. Floro, W. B. Gauster, R. Q. Hwang, B. Swartzentruber, J. Y. Tsao
(505) 844-8951 01-3 $333,000

Advanced growth techniques are studied for the synthesis of improved semiconductor and thin film structures. Studies concentrate on Si and Ge and layered III-V compounds. In situ diagnostics are used in conjunction with molecular beam epitaxy (MBE) and novel growth method to grow new semiconductor structures. A primary purpose of this research is to provide new understanding of fundamental thin film growth mechanisms and new methods and diagnostics for the growth of improved epitaxial layered structures. Advanced in situ techniques yield surface structure, film stress, composition and chemical reactivity information. Real-time studies enable us to efficiently explore the interaction between film properties and processing parameters. Theoretical studies model the growth processes and address growth mechanisms in order to interpret and guide the experimental studies.

245. ENERGETIC-PARTICLE SYNTHESIS AND SCIENCE OF MATERIALS
S. M. Myers, J. C. Barbour, M. T. Dugger, D. M. Follstaedt, J. A. Knapp, C. H. Seager, W. R. Wampler
(505) 844-6076 01-3 $732,000

Superior new materials are synthesized and mechanistically characterized using ion beams, pulsed laser deposition, and electron-cyclotron-resonance plasmas. Additionally, fundamental studies employing energetic-particle techniques provide new understanding of the atomic processes and microstructures that govern materials properties. Representative areas of research include the formation of new Al, Fe, and Ni alloys with very high strength and enhanced tribological properties, the synthesis and understanding of the atomic processes and microstructures that govern materials properties. Representative areas of research include the formation of new Al, Fe, and Ni alloys with very high strength and enhanced tribological properties, the synthesis and understanding of improved dielectrics, identification and mechanistic characterization of new trapping mechanisms for detrimental impurities in semiconductors, and fundamental studies of the interactions of H with semiconductors. This program participates in the focus project on Surface Hardness of the Department of Energy's Center of Excellence in Synthesis and Processing of Advanced Materials.

246. ARTIFICIALLY STRUCTURED SEMICONDUCTORS
P. L. Gourley, E. D. Jones, S. K. Lyo, J. S. Nelson, M. B. Sinclair
(505) 844-5806 01-5 $430,000

Compound semiconductor heterostructures, quantum wells and surface-structured materials to explore solutions to new and existing semiconductor materials problems. Theoretical and experimental understanding of semiconductor physics and materials science to produce new semiconductor materials with useful electronic properties not available in bulk compound semiconductor crystals. Fundamental material properties including band structure, electronic transport, crystal stability, optical transitions, and nonlinear optical properties. The materials applications for high speed switching, photovoltaics, optical detectors, lasers, and efficient high generators.

247. METAL-CERAMICS INTERFACIAL REACTIONS
R. E. Loehman, K. G. Ewsuk, T. Swiler (Univ. of NM), A. P. Tomsai (BNL)
(505) 272-7601 01-5 $334,000

Fundamental understanding of the interfacial reactions of molten aluminum and aluminum alloys with other materials at high temperatures. Predictive model for reactive wetting of oxides by aluminum and aluminum alloys. Quantify processes at Al-ceramic interfaces. Improved refractories and metal process equipment, better mold releases, protective coatings, die lubricants, hardfacing for high wear rate applications, and improved techniques for aluminum joining. Lower cost of lightweight materials and improvement of properties.

248. FIELD-STRUCTURED ANISOTROPIC COMPOSITES
J. E. Martin, R. A. Anderson, C. P. Tigges
(505) 844-9125 01-5 $156,000

This program will develop the modeling, synthesis, and processing capability to create novel, tailorable anisotropic polymer/ceramic and polymer/metal composite materials. External electric or magnetic fields to systems consisting of a polymerizable continuous phase into which particles having an electric permittivity or magnetic permeability mismatch are suspended. These materials are expected to find a variety of applications capitalizing on their anisotropic electrical and mechanical properties.

Solid State Physics - 02 -

249. SPONTANEOUS COMPOSITION MODULATION IN COMPOUND SEMICONDUCTORS
E. D. Jones, D. M. Follstaedt, S. Lee, J. L. Reno
(505) 844-8752 02-2 $190,000

Investigate the fundamental properties and origins of spontaneous composition modulation in compound semiconductor epilayers and superlattices as part of a joint NREL/Sandia BES collaboration. The program depends on state-of-the-art semiconductor physics, surface physics, instrumentation measurement science, and materials science in order to develop new and exciting semiconductor properties not found in nature. This program investigates such material properties as band structure, optical response, growth parameters, and surface induced effects. Advanced characterization techniques are developed for rapid sample characterization. Theoretical as well as experimental understandings are required. The materials under study potentially have a high impact in the areas of high efficiency photovoltaic devices, polarized-laser applications, short-gate field effect transistors.

250. TAILORED SURFACES AND INTERFACES FOR MATERIALS APPLICATIONS
G. L. Kellogg, P. J. Feibelman, T. M. Mayer, B. Swartzentruber
(505) 844-2079 02-2 $497,000

The goals of this program are to understand the microscopic mechanisms that control the growth of thin surface films and to use this knowledge to develop predictive models for materials synthesis. Atomic-scale processes involving adatoms, vacancies, steps, and impurities play a key role in how a crystal or epitaxial film grows. We are conducting experimental and modeling studies to address the fundamental interactions associated with these kinetic processes. Our current emphasis is on achieving a fundamental understanding of how foreign atoms or "surfactants" modify nucleation and growth and control the evolution of surface and interface morphology. Combined with studies of chemically mediated nucleation during chemical vapor deposition (CVD). These studies will enable the development of a science-based approach to the fabrication of materials for improved mechanical performance, chemical reactivity, corrosion resistance, and magnetic and electronic properties.

251. MATERIALS SCIENCE AND PHYSICS OF TL-BA-CA-CU-O SUPERCONDUCTORS
E. L. Venturini, B. Morosin, P. P. Newcomer, M. P. Siegal
(505) 844-7055 02-2 $477,000

This program focuses on the fundamental physical properties of the cuprate-based high-temperature superconductors with emphasis on thin films of the thallium system. The primary goal is a detailed understanding of structure/property relationships, particularly the effects of synthesis conditions, structural phase, cation and oxygen stoichiometry and lattice defects on the superconducting transition temperature, critical current density and vortex pinning. Diagnostic and processing capabilities include magnetic studies of critical current and vortex dynamics at high magnetic fields in the presence of tailored nanoscale defects generated by high-energy, heavy-ion irradiation or other methods. Active internal and external collaborations complement our expanding knowledge of these challenging materials.

252. TRANSPORT IN UNCONVENTIONAL SOLIDS
T. L. Aselage, D. Emin, S. S. McCready, G. A. Samara, D. R. Tallant
(505) 845-8027 02-5 $448,000

This program investigates solids whose bonding and/or structures promote unusually strong interactions between charge carriers and their surrounding atoms. As a result of these interactions, electronic transport in unconventional solids is distinct from solids in which charge carriers move quasi-freely. Boron-rich solids, clathrate networks, conducting and superconducting oxides, and polymers are among the materials that are being examined. High-quality samples are synthesized by a variety of techniques. Electrical transport properties are measured over an exceptionally wide temperature range. Facilities for transport measurements over a temperature range of 4-1800 K and in magnetic fields as large as 10T are employed. Our understanding of transport mechanisms is enhanced through complementary studies of the structures, vibrations, and optical, dielectric, and magnetic properties of the materials. Insights garnered from this work suggest distinctive applications, including novel, high-efficiency thermoelectrics, unique energy conversion devices, and solid state neutron detectors.

Materials Chemistry - 03 -

253. CHEMICAL VAPOR DEPOSITION
M. E. Coltrin, M. E. Bartram, W. G. Breiland, J. R. Creighton, J. Han, P. Ho, H. K. Moffat, J. Y. Tsao
(505) 844-7843 03-3 $625,000

Studies of important vapor-phase and surface reactions during CVD under conditions used to fabricate photovoltaic cells, wear- and corrosion-resistant coatings, and semiconductor thin films. Measurements of major and minor species densities, gas temperatures and flow fields using laser Raman spectroscopy, laser-induced fluorescence, and laser velocimetry. Development of predictive numerical models of the coupled chemical kinetics and transport. Application of a wide array of UHV, molecular beam, and in situ measurement capabilities to study surface reactions, monitor growth, and study the product materials.

254. SYNTHESIS AND PROCESSING OF NANOCLUSTERS FOR ENERGY APPLICATIONS
J. P. Wilcoxon, J. E. Martin, T. Thurston
(505) 844-3939 03-3 $269,000

The work exploits a unique micellar synthesis method to create new size-controlled metal and semiconductor nanoclusters and investigate those physical properties germane to energy applications. The most promising applications are in catalysis and photocatalysis, so emphasis is on materials for these applications. Metal clusters from base metals are being examined as candidates for replacing precious transition metals for coal liquefaction and other reactions. The catalytic activity of these clusters will be evaluated in model hydrogenation reactions. The work also investigates the use of semiconductor nanoclusters to efficiently create electron-hole pairs for photocatalysis and then bind reducing and oxidizing nanoclusters to the semiconductors to create cluster assemblies that can convert sunlight to chemical fuels.

STANFORD SYNCHROTRON RADIATION LABORATORY

Stanford University
Stanford, CA 94309-0210

K. O. Hodgson - (650) 926-3153
Fax: (650) 926-4100

Facility Operations - 04 -

255. RESEARCH AND DEVELOPMENT OF SYNCHROTRON RADIATION FACILITIES
K. O. Hodgson
(415) 926-3153 04-1 $3,650,000

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, studies of highly perfect semiconductor crystals using X-ray topography, analysis of microcontamination on silicon wafer surfaces, photoemission studies of superconductors and semiconductor interfaces (e.g., heterojunctions and Schottky barriers), photoemission studies of highly correlated materials including magnetic systems, metal surfaces (especially catalytic reactions on surfaces) and development of techniques such as surface EXAFS, photoelectron diffraction, and interface studies using core level spectroscopy. Photoelectron and X-ray absorption spectroscopic studies of catalysts. R&D on the design, development and improvement of accelerators and insertion devices for synchrotron radiation production. Design and development of short wavelength free electron lasers and high performance photocathode guns. Development of Laue diffraction for time-resolved protein crystallography. Development of X-ray absorption spectroscopy methods to study the speciation of environmentally important materials and contaminants. Research in utilization of X-ray absorption edges to determine electronic structure of metal complexes. Application of X-ray absorption spectroscopy to the study of biological systems.

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 AT BIRMINGHAM
Birmingham, AL 34294-0111

256. THE ALABAMA DOE/EPSCOR PROGRAM
K. M. Pruitt
(205) 934-4346 05-1 $750,000

The Alabama DOE/EPSCoR project will conduct research in three cluster areas: petroleum reservoir characterization, fusion energy, and novel organic semiconducting materials. The petroleum reservoir characterization team seeks to maximize petroleum recovery by constructing a geological model from depositional, digentic, structural and pore-fluid studies; performing reservoir engineering analyses and simulations using simulation history matching techniques; and applying neural networks to develop methods for automoatic determination of reservoir flow units. Alabama's fusion energy cluster is helping advance the science community's understanding of fundamental issues related to plasma confinement, heating, and atomic physics. A major objective of the cluster's program is to design a quasi-symmetric stellarator optimized for improved plasma confinement. Finally, projects undertaken by the novel organic semiconductor materials group focus on the electronic and optical properties of materials and include studies on the synthesis and characterization of molecules and polymers with applications in photovoltaics, optical switches, and modulators.

ALFRED UNIVERSITY
2 Pine Street
Alfred, NY 14802

257. STRUCTURE, STOICHIOMETRY AND STABILITY IN MAGNETOPLUMBITE AND β-ALUMINA TYPE CERAMICS
A. N. Cormack, Department of Ceramic Science and Engineering
(607) 871-2422 01-1 $100,170

Atomistic simulation of defect structures and energies for defect clusters in mirror planes of hexa-aluminates ($MA_{12}O_{19}$) with magnetoplumbite and beta-alumina structures; defect cluster interaction. Born model with Buckingham potential and shell model treatment of atomic polarizations; atomic relaxation treated by Mott-Littleton approximation. Further investigation of barium hexa-aluminates to interpret recent unexplained experimental results; investigation of effects of lanthanide doping on structural stability and defect chemistry; investigation of possible mixed alkali or alkaline earth effects; investigation of structural basis for high Na^+ conductivity in hypostoichiometric β-alumina; development of appropriate interatomic potentials for Ag and investigation of Ag hexa-aluminates; investigation of possible O_2-ion conducting in β-alumina; investigation of Li^+ as a structural stabilizer; investigation of the incorporation of transition metal dopants.

ARIZONA STATE UNIVERSITY
Tempe, AZ 85287

258. POLYMER-IN-SALT ("IONIC RUBBER") FAST ION ELECTROLYTES AND RELATED MATERIALS
C. A. Angell, Department of Chemistry
(602) 965-7217 01-1 $89,648

Investigation of polymer-in-salt compounds for use as solid electrolytes in high energy density batteries. A variety of ambient temperature molten salts, rubberized by the addition of polymers will be examined in order to establish materials with a single ion conductivity high enough to serve as a battery electrolyte and with a sufficiently low glass transition temperature that the material remains amorphous. The work will require improvements in both the salt constitution and polymer type; modifications of the materials with solid particulates; materials having a polymer matrix forming network that supports an ionic phase; and the necessary physical measurements to characterize these materials.

259. PLANAR INTERFACES: SYNTHESIS FOR HIGH RESOLUTION CHEMISTRY AND STRUCTURE ANALYSIS
R.W. Carpenter, Center for Solid State Science
(602) 965-4549

S. H. Lin, Department of Chemistry
(602) 965-4549 01-1 $101,010

High spatial resolution analytical electron microscopy investigation of compositional gradients and solute segregation at interfaces and grain boundaries in ceramic/ceramic and ceramic/metal systems. Relationships between chemical and structural width of interfaces and boundaries studied as functions of material system and temperature. Theoretical analysis of interfaces and boundaries using quantum molecular dynamic computational methods.

UNIVERSITY OF ARIZONA
Tucson, AZ 85721

260. EARLY STAGES OF NUCLEATION

M.C. Weinberg, Department of Materials Science and Engineering
(602) 621-6909 01-1 $102,270

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

261. CONTROL OF MICROSTRUCTURE ON FATIGUE IN ALUMINUM AUTOMOTIVE CASTINGS

D. Poirier, Department of Materials Science and Engineering
(520) 621-6072 01-5 $405,000

Investigation of structure-property relationships in fatigue behavior of aluminum alloys. Effects of microporosity on fatigue resistances will be studied with alloy A356.2 (Al-7%Si-0.3&Mg) which will be produced as near-net-shape castings using pressure-riseless casting/vacuum-riserless casting (PRC/VRC). Effects of pore-size, hydrogen content, strontium modification, and grain refiners will be studied with Al-Ti-B and Al-Ti-C alloys. Effects of near-surface microshrinkage, secondary dendrite arm spacing, and inclusions and undissolved second-phase particles on fatigue crack propagation and fracture toughness measurements will be determined. An improved process model will be developed which will take into account pore formation and solidification shrinkage. An experimental apparatus utilizing acoustic emission will be developed to detect nucleation and early growth of pores. Casting of alloys will be performed collaboratively by the Alcoa Technical Center.

262. ARTIFICIALLY STRUCTURED MAGNETIC MATERIALS

C. M. Falco, Department of Physics
(602) 621-6771

B. N. Engel, Department of Physics
(602) 621-6771 02-2 $90,000

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

BOSTON COLLEGE
Chestnut Hill, MA 02167

263. MANY-BODY THEORY OF THE METAL-INSULATOR TRANSITION IN HIGH MAGNETIC FIELDS

K. S. Bedell, Department of Physics
(617) 552-3575 02-3 $49,996

The metal-insulator transition is to be studied utilizing the model of a local Fermi liquid theory. The transition will be studied for cubic Perovskites ($La_{1-x}A_xTiO_3$; A=Ca,Sr) in the presence of intense magnetic fields. Collossal magnetoresistance will be modeled by coupling the local Fermi liquid conduction electrons to a set of localized ferromagnetically ordered spins. A local Fermi liquid sytem which is restricted to be ferromagnetic will also be investigated. Both the micrscopic conditions for, and the properties of, such a constrained system will be sought.

BOSTON UNIVERSITY
590 Commonwealth Avenue
Boston, MA 02215

264. STUDIES OF THE STRUCTURE & DYNAMICS OF THE SURFACE SPIN SYSTEMS OF MAGNETIC GROWTH TRENDS OF TRANSITION METAL OVERLAYERS, USING HE SPECTROSCOPIES
M. M. El-Batanouny, Department of Physics
(617) 353-4721 02-4 $150,000

Use of scattered spin-polarized metastable He(2^3S) atoms from surfaces both elastically and inelastically, to study the structural, dynamic and magnetic trends of the 3D transition metal overlayers-Cu, Au, Ag and Cr on Pd(111) and Pd(110) substrates; and Pd and Cu on Nb(110) substrate. Magnetic properties will be studied in the newly constructed Spin-Polarized Metastable He (SMPH) facility. Spin-ordering in NiO, MnO and C_oO will be investigated. Large-scale canonical molecular dynamics simulations combining a hybrid Nose-Hoover thermostat and Andersen's constant pressure algorithms will parallel the experiments.

BRANDEIS UNIVERSITY
Waltham, MA 02254

265. INTERMETALLIC ALLOYS: PATTERNS AND COMPLEXITY
B. Chakraborty, Department of Physics
(617) 736-2835 01-1 $76,711

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

266. ELECTRIC FIELD-INDUCED INTERACTIONS IN COLLOIDAL SUSPENSIONS AND THE STRUCTURE OF ELECTRORHEOLOGICAL FLUIDS
S. Fraden, Department of Physics
(617) 736-2835 01-3 $98,706

Electric field-induced interactions between colloidal particles and structure of electro-rheological fluids, spatial organizational of colloids in external electric fields and shear flows. Neutral colloids in insulating solvents, silica spheres in organic solvents such as chloroform; charged colloids in conducting solvents, polystyrene spheres in aqueous suspensions. Colloidal interaction and structure in electric field and no shear flow; effects of field strength and frequency; field-induced interparticle potential; test of model of electro-hydrodynamic stability; liquid-to-crystal phase transitions as function field strength and particle concentration; electric field-induced ordering of concentrated colloidal suspensions. Structure of colloids in shear flow in absence of electric fields; simultaneous direct visualization and light scattering. Structure of colloids in combined shear flow and electric fields.

267. ULTRA HIGH RESOLUTION ARP SPECTROMETER SYSTEM FOR NSLS UNDULATOR BEAMLINE U13
E. S. Jensen, Physics Department
(617) 736-2835 02-2 $120,000

Development of an ultra-high resolution angular resolved photoemission spectrometer for use on Beamline U13 at the National Synchrotron Light Source.

BROWN UNIVERSITY
Providence, RI 02912

268. IN SITU TRANSMISSION ELECTRON MICROSCOPY INVESTIGATION OF SINTERING AND RELATED PHENOMENA IN CERAMIC PARTICLES
J. Rankin, Department of Engineering
(401) 863-2637 01-1 $109,949

In-situ TEM study of sintering and related phenomena in ceramic oxides. Sintering of nanosized single-crystal cubes of MgO for the determination of neck stability and coalescence criteria. Sintering of constrained and unconstrained systems for the study of particle reorientation during heating. Chemical reactions during sintering and the role of chemical modification for the suppression of grain growth. In-situ observations of the growth of atoms or clusters on ceramic surfaces.

269. GRAIN BOUNDARY STRUCTURE, SEGREGATION, AND SLIDING
C. Briant, Division of Engineering
(401) 863-2626 01-2 $98,000

Experimental and modeling study of grain boundary structure, segregation and sliding in Al. Tilt bicrystals prepared via Bridgman technique. Experimental studies using orientation imaging microscopy and HRTEM. Tilt boundaries in Al examined using embedded atom modeling in conjunction with high-resolution image simulation. Structural evolution in Cu-Ni and Cu-Bi as a function of segregant concentration for high angle, low coincidence structures using Monte Carlo simulations. Auger spectroscopy and EELS. Static energy and embedded atom modeling and HRTEM examination of grain boundary sliding in Al and Cu-Bi, Cu-Ni systems.

270. SURFACES AND THIN FILMS STUDIED BY PICOSECOND ULTRASONICS

H. J. Maris, Department of Physics
(401) 863-2185

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

Thin films, interfaces, and superlattices investigated using very high frequency (10-700GHz) ultrasonics. The ultrasound is produced by short (< 1 picosecond) laser pulses impinging on a thin metallic layer. Fundamental studies of lattice dynamics, relaxation phenomena, absorbtion phenomena, and diffusion phenomena both in bulk and at interfaces.

UNIVERSITY OF CALIFORNIA AT DAVIS
Davis, CA 95616-5294

271. THERMOCHEMICAL STUDIES OF THE STABILITY OF NITRIDES AND OXYNITRIDES

A. Navrotsky, Department of Chemical Engineering and Materials Science
(916) 752-2075 01-3 $95,233

The basic thermodynamic properties of nitrides and oxynitrides and the relations among energetics, structure, and bonding are far less well known than for oxides. The goals of this work are to develop high temperature reaction calorimetric techniques for measuring enthalpies of formation of nitrides and oxynitrides, to determine energetics of sialons and ternary nitrides, and to formulate thermochemical systematics useful for predicting phase stability, materials compatability, and the synthesis of new compounds.

272. DEVELOPMENT OF NEXT-GENERATION DETECTORS AND INSTRUMENTATION FOR PHOTOELECTRON SPECTROSCOPY, DIFFRACTION AND HOLOGRAPHY

C. Fadley, Physics Department
(916) 752-8788 02-2 $247,465

A new multichannel detector and a next-generation sample goniometer for use in photoelectron spectroscopy will be developed. The new detector will enable the full utilization of the high-brightness radiation generated by the Advanced Light Source at Lawrence Berkeley National Laboratory and can be used at other third generation synchrotron radiation sources as well. The goniometer will permit equally rapid scanning of specimen angles or photon energies for angle-resolved photoemission studies, photoelectron diffraction and photoelectron holography measurements. In addition, new software and hardware will be developed to permit rapid and accurate photoelectron spectra collection and analysis.

273. THEORIES OF THE HEAVY FERMION NORMAL STATE

D. L. Cox, Physics Department
(916) 752-1789 02-3 $55,000 (9 months)

The normal state properties of heavy fermion materials are studied. Emphasis is in three areas: (i) Monte Carlo studies of the two-channel Kondo lattice in infinite dimensions. Interest in the possible non-Fermi liquid behavior and precision of simpler approximations. (ii) Model uranium impurities in the extreme mixed valence phase where f^2 and f^3 configurations are nearly equally occupied. Interest is the crossover between ground state nature and implications for the non-linear susceptibility. (iii) Melting of local density approximation calculations of hybridization matrix elements and host electronic structure with dynamic many body treatments of the f-electron sites.

UNIVERSITY OF CALIFORNIA AT IRVINE
Irvine, CA 92717

274. THEORETICAL STUDIES OF ELECTRON SCATTERING SPECTROSCOPIES OF MAGNETIC SURFACES AND ULTRA THIN FILMS

D. L. Mills, Department of Physics
(714) 824-5148 02-3 $94,000

Theory of the inelastic scattering of electrons, ions, and neutral atoms from elementary excitations at surfaces, and the development of theoretical descriptions of these excitations. Emphasis on electron energy loss from surface phonons at both clean and adsorbate-covered surfaces. Studies of spin-flip scattering of low energy electrons from magnetic excitations at surfaces, and excitation of surface phonons by helium atoms. Strong emphasis on the quantitative comparison between the results of this program and experimental data. Tightly coupled effort between Professor Mills and Professor Tong at the University of Wisconsin at Milwaukee.

275. OPTICAL SPECTROSCOPY AND STM STUDIES OF MOLECULAR ADSORBATES AND ANISOTROPICULTRATHIN FILMS

J.C. Hemminger, Department of Chemistry
(714) 824-6020 03-2 $120,000

Temperature dependant scanning tunnelling microscopy (STM) will be used in conjunction with both optical probes (e.g., Raman spectroscopy and laser induced thermal desorption spectroscopy) and conventional UHV analytical techniques (e.g., Auger electron spectroscopy, X-ray photoemission spectroscopy and low energy electron diffraction) to investigate anisotropic thin films of organic molecules. Emphasis will be placed on controlling the preparation of such films. The effects of substrate structure (e.g., surface steps) on adsorbate orientation will be of particular interest.

UNIVERSITY OF CALIFORNIA AT LOS ANGELES
6532 Boelter Hall
Los Angeles, CA 90025-1595

276. EVOLUTION OF GAMMA' (NI_3X) PRECIPITATION KINETICS, MORPHOLOGY AND SPATIAL CORRELATIONS IN NI-BASE ALLOYS AGED UNDER EXTERNALLY APPLIED STRESS

A.J. Ardell, Department of Materials Science and Engineering
(310) 825-7011 01-2 $98,000

Kinetics studies of coarsening of gamma' precipitates Ni_3X (X is solute atom) during aging under stress and hydrostatic pressure. The formation of these stress induced precipitates is key to the toughening of the nickel based superalloys.

277. UNIVERSAL RELATION BETWEEN LONGITUDINAL AND TRANSVERSE CONDUCTIVITIES AND VARIATIONAL ANALYSIS OF WIGNER CRYSTAL STATES IN QUANTUM HALL EFFECT

S. Feng, Physics Department
(310) 825-8530 02-3 $0 (0 months)

The relation of the Hall conductance sigmaxy and the longitudinal conductance sigmaxx in the inter-plateau region will be investigated. The usual assumption that all dynamic effects occur at the edges of the material will be checked by using a model that incorporates electron-electron interactions. The importance of residual effects in the bulk of the material will be investigated.

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

278. GROWTH INDUCED MAGNETIC ANISOTROPY IN AMORPHOUS THIN FILMS

F. Hellman, Department of Physics
(619) 534-5533 02-2 $85,000

The relationships among macroscopic magnetic anisotropy, structural anisotropy and the vapor deposition growth process in amorphous thin films of rare earth transition metal alloys is being examined. Experimental observations are compared to models describing the effects of growth parameters on film properties. Magnetic, thermodynamic and structural measurements are used to determine magnetic phase diagrams and to test theoretical predictions for random magnetic materials in the presence of controlled macroscopic anisotropy.

279. SUPERCONDUCTIVITY AND MAGNETISM IN D- AND F-ELECTRON MATERIALS

M. B. Maple, Department of Physics
(619) 534-3968 02-2 $317,500

Research on superconductivity, magnetism, and the mutual interaction of these two phenomena in d- and f-electron materials will be carried out. The emphasis of the research will be on: 1) high T_c copper oxide superconductors and other novel superconducting materials such as the recently discovered lanthanide-transition metal-boride-carbide superconductors, and 2) investigation of the anisotropic normal and superconducting state properties of these materials as a function of doping, oxygen vacancy concentration, pressure and magnetic field. The goals are to elucidate the type of electron pairing involved in the superconductivity, to characterize the properties important to technological applications, and to explore new methods of fabricating high T_c superconducting composites.

280. PREPARATION AND CHARACTERIZATION OF SUPERLATTICES

I. K. Schuller, Department of Physics
(619) 534-2540 02-2 $100,000

Preparation and characterization, both during and after growth, of novel microstructures and exploration of novel physical properties produced by new geometries. A combined thin film and electron beam lithography technique is used to prepare model systems which allow the development of new characterization techniques, or to prepare new systems with interesting physical properties. Model systems include samples such as superlattices, vicinally cut crystals, narrow lines and dots in a variety of configurations. New microstructures are combined to prepare and investigate new properties such as exchange bias in ferromagnetic-antiferromagnetic bilayers, magnetic coercivity in single and multilayered films, and magnetic dots.

UNIVERSITY OF CALIFORNIA AT SANTA BARBARA
Santa Barbara, CA 93106

281. THEORIES OF PATTERN FORMATION AND NONEQUILIBRIUM PHENOMENA IN MATERIALS

J. S. Langer, Department of Physics
(805) 893-2280 02-3 $110,296

Theoretical investigations of phenomena that occur in systems far from thermodynamic or mechanical equilibrium; dynamic fracture; kinetics of phase separation. Dynamic stability analyses; mechanics of the cohesive (or "process") zone; effects of dissipative mechanisms; physical origin of stresses that resist crack bending; brittle solids; nonlinear processes. Effects of shear on phase separation in multicomponent viscous fluids; theory of localize failure; comparative stability of competing precipitation patterns; coarsening mechanisms.

282. NUMERICAL SIMULATION OF QUANTUM MANY-BODY SYSTEMS

D. J. Scalapino, Department of Physics
(805) 893-2871

R. T. Sugar, Department of Physics
(805) 893-3469 02-3 $80,000

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

283. MOLECULAR PROPERTIES OF THIN ORGANIC INTERFACIAL FILMS

J. Israelachvili, Department of Chemical and Nuclear Engineering
(805) 893-3412 03-1 $305,000

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

UNIVERSITY OF CALIFORNIA AT SANTA CRUZ
1156 High Street
Santa Cruz, CA 95064

284. STATICS AND DYNAMICS IN SYSTEMS WITH FRUSTRATION AND/OR RANDOMNESS
D. Belanger, Department of Physics
(408) 459-2871 02-1 $90,000

Neutron scattering, optical birefringence, Faraday rotation, and pulsed specific heat techniques will be applied to magnetic systems with frustrated interactions and/or random interactions. Epitaxial films are used to complement bulk samples: Thin films are used in neutron scattering to avoid extinction effects. Epitaxial multilayers are used to explore crossover from three dimensional to two dimensional behavior. Materials studied include: $Fe_xZn_{1-x}F_2$, $Mn_xZn_{1-x}F_2$, $Rb_2Co_xMg_{1-x}F_4$, $FeBr_2$, UNi_4B.

CALIFORNIA INSTITUTE OF TECHNOLOGY
138-78
Pasadena, CA 91125

285. METASTABLE ALLOY STRUCTURES AND PROPERTIES
W. L. Johnson, Department of Material Science
(818) 395-4433 01-1 $396,851

Development of alloy compositions which favor formation of bulk metallic glasses, and the design and construction of new equipment for the production of high quality bulk metallic glass samples. Thermodynamic and kinetic studies of these new materials using a combination of various processing methods (levitation melting, etc.) together with calorimetry studies and microstructural analysis. Work focuses on the thermodynamic functions such as heat capacity and on studies on atomic diffusion, viscosity, and the glass transition. Mechanical property studies include measurements of elastic constants, studies of the dynamic deformation behavior using such methods as Hopkinson bar tests. Techniques include electron microscopy, X-ray diffraction, small angle X-ray diffraction, and neutron and electron diffraction. Molecular dynamic methods will be used to carry out atomistic simulations of the properties of metallic glasses.

286. CALORIMETRY AND INELASTIC SCATTERING STUDIES OF THE VIBRATIONAL ENTROPY OF ALLOY PHASES
B. Fultz, Materials Science Department
(818) 395-2170 01-3 $99,832

Measurement of vibrational entropy differences between different alloy phases by precision cryogenic differential calorimetry. Alloys of interest include DO3; Fe_3Si, Fe_3Ge, and Ll_2; Au_3Cu, Cu_3Au, for unmixing alloys such as bcc Fe-50%Cr, bcc Fe-25%Sn, bcc Fe20%Cu, bcc and fcc Fe-50%Cu, fcc Ag-50%Cu. Phonon density of state measurements using neutrons and synchrotron radiation. Incoherent inelastic neutron scattering measurements on different phases of alloys of V, Co, and Ni. A new technique based on inelastic nuclear resonant gamma-ray scattering will be used for measuring the phonon partial density of states of 57Fe atoms.

CARNEGIE MELLON UNIVERSITY
Pittsburgh, PA 15213

287. THE ROLE OF MICROSTRUCTURAL PHENOMENA IN MAGNETIC MATERIALS
D. E. Laughlin, Department of Materials Science and Engineering
(412) 268-2706

N. Lambeth, Department of Materials Science and Engineering
(412) 268-3674 01-1 $83,413

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

288. MELTING, FREEZING AND ROUGHENING AT SOLID/SOLID AND LIQUID/SOLID INTERFACES
P. Wynblatt, Department of Materials Science and Engineering
(412) 268-8711 01-1 $94,893

The research intends to extend previous knowledge gained on the behavior of interphase boundaries in alloy systems to solid/solid and liquid/solid interfaces. Interfacial energy, and its control by means of segregation phenomena, at lead/aluminum interfaces will be studied. This system has been selected so as to avoid the possibility of interfacial reactions which could lead to the formation of brittle reaction products. Monte Carlo simulations using extended atom-like potentials will augment the experimental studies.

289. MECHANISMS OF DEFORMATION IN B2 ALUMINIDES

T.M. Pollock, Department of Materials Science and Engineering
(412) 268-2973 01-2 $99,738

Study of the fundamental deformation mechanisms in three B2 aluminide systems; NiAl, FeAl, and RuAl. Measurement of strain rate sensitivities, activation volumes and activation energies. Dislocation dynamics at low temperature; compression experiments; effect of solute additions; TEM observations of dislocation microstructures for mechanical property correlations.

CASE WESTERN RESERVE UNIVERSITY
10900 Euclid Avenue
Cleveland, OH 44106

290. POLYTYPIC TRANSFORMATIONS IN SIC AND GAN

P. Pirouz, Department of Materials Science and Engineering
(216) 368-6486 01-1 $126,517

Experimental and theoretical study of mechanisms for polytypic transformations of alpha-SiC and GaN. Compressive deformation of 6H-SiC single crystals at temperatures up to 1700^0, inert atmospheres and nitrogen environments; TEM observation of deformation modes and polytype development. Annealing experiments on 6H-SiC single crystals and 3C-SiC films; inert gas and nitrogen environments; effects of dislocations introduced by surface scratches investigated; TEM determination of polytype development. Determination of the presence of residual dislocations on cross-slip planes following polytypic transformation; thick sections examined by HVEM. Theoretical analysis of formation of Frank-Read dislocation loops and cross-slip of dissociated screw dislocations, effects of stress and temperature; quantitative analysis ofmechanism of cross-slip; determination of the activation energy for themotion of partial dislocations.

CENTER FOR ENVIRONMENTAL SCIENCES & ENGINEERING
1664 N. Virginia Street
Reno, NV 89557-0187

291. NEVADA DOE EPSCOR PROGRAM FOR THE STIMULATION OF EXPERIMENTAL PROGRAM COMPETITIVE RESEARCH (EPSCOR)

J. N. Seiber
(702) 784-6460 05-1 $750,000

The Nevada DOE/EPSCoR program continues to enhance the State's research competitiveness in energy-related areas of chemical physics and in studies of the environment's response to increased atmospheric carbon dioxide. The chemical physics efforts of Research Cluster 1 are divided into three project areas: laser and ion physics, synchrotron radiation, and nanostructures. The laser and ion physics effort involves the development of a multi-charged ion beam facility at the University of Nevada-Reno and a collaboration with EBIT, a hot highly-charged plasma source at Lawrence Livermore National Laboratory. The Synchrotron Radiation project is a multifaceted research program that brings together a team of 17 experimental and theoretical groups interested in X-ray atomic and molecular spectroscopy using synchrotron radiation from the Advanced Light Source at the Lawrence Berkeley National Laboratory. The major focus of the effort is to understand the processes that govern X-ray interactions with atoms and molecules. The nanostructures project is a partnership in condensed-matter physics between a theoretical effort at the University of Nevada, Las Vegas, and an experimental effort at Los Alamos National Laboratory. The primary objective of the project is to develop a systematic first-principles study of the novel properties of nanometer-sized mateials systems. Research Cluster 2, titled "Plant Responses to CO_2," is testing a series of hypotheses on the response of desert vegetation to increased atmospheric CO_2. The effort spans the levels of biological integration from cellular to ecosystem.

UNIVERSITY OF CHICAGO
5640 S. Ellis Avenue
Chicago, IL 60637

292. HIGH-TEMPERATURE THERMOCHEMISTRY OF TRANSITION METAL BORIDES, SILICIDES AND RELATED COMPOUNDS

O. J. Kleppa, The James Franck Institute
(773) 702-7198 01-3 $78,195

Studies of the enthalpies of formation of the lanthanum borides, carbides, silicides, germanides, and stannides. The investigations based on the application of direct synthesis calorimetry. The work on the lanthanides will be extended to the corresponding compounds formed be the actinides Th and U. New studies of transition metal carbides, gallides and stannides.

UNIVERSITY OF CINCINNATI
P.O Box 210012
Cincinnati, OH 45221-0012

293. ROLE OF INTERFACIAL PROPERTIES ON THE MATRIX CRACKING AND CREEP BEHAVIORS IN CERAMIC-MATRIX COMPOSITES

R. N. Singh, Department of Materials Science and Engineering
(513) 556-5172 01-5 $93,962

Mechanical properties of fiber-reinforced ceramic composites at elevated temperatures. Matrix cracking and creep behaviors of composites. Analytical models of mechanical response to composites. Fabrication of composites with tailored microstructure, flaw size, fiber architecture, and interfacial properties. Role of interfacial properties and flaw size on the first-matrix cracking and creep behaviors at elevated temperatures.

CITY UNIVERSITY OF NEW YORK (LEHMAN COLLEGE)
250 Bedford Park Blvd W.
Bronx, NY 10468-1589

294. STATICS AND DYNAMICS OF THE MAGNETIC FLUX IN HIGH TEMPERATURE SUPERCONDUCTORS

E. M. Chudnovsky, Department of Physics and Astronomy
(718) 960-8770 02-3 $40,000

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

CITY UNIVERSITY OF NEW YORK AT CITY COLLEGE
Convent Ave. & 138th St.
New York, NY 10031

295. NONLINEAR DYNAMICS AND PATTERN SELECTION AT THE CRYSTAL - MELT INTERFACE

H. Z. Cummins, Department of Physics
(212) 650-6921 02-2 $55,000

Dynamics and pattern formation at the crystal-melt interface during solidification. Focus on growth of fluctuations, dendritic growth, effect of perturbations on dendritic sidebranching. Particular interest in the instability to the spacial period doubling occurring when the wavelength of a periodic modulation is too short. Initial transient conditions are studied rather than steady state demonstrating history effects. Investigations conducted utilizing light scattering, videomicroscopy, and fluorescence techniques. Laser pulses are used to produce either local or sinusoidal thermal perturbations on the crystal growth process.

296. TRANSPORT STUDIES IN HEAVILY DOPED SEMICONDUCTORS

M. P. Sarachik, Department of Physics
(212) 650-5618 02-2 $85,000

Investigation of the properties of doped semiconductors which undergo a transition from insulating to metallic behavior with increasing dopant concentration. Examination of the role of disorder and correlations on the transition. Uniaxial stress and dopant concentration will be used totune materials through the transition. Determination of the effect of spin-orbit scattering, spin-flip scattering, magnetic field, quantum interference phenomena, and Coulomb correlations and exchange. Experiments will include measurements of resistivity, Hall coefficient and dielectric constant of CdSe:In and of Si:B, Si:P.

297. OPTICAL INTERACTIONS IN MICROSTRUCTURES

M. Lax, Department of Physics
(212) 650-6864 02-3 $40,000 (10 months)

Theoretical investigations of electrons confirmed by a potential barrier in two dimensions interacting with freely propagating phonons. Time dependent transport effects in the femto-second regime. Inelastic tunneling through barriers, including screening and 3-D effects. Ultra fast relaxation of photo-excited electrons study of the phonon mediated nonlinear optical response of quasi 2-D polymeric systems including homogeneously and inhomogeneously broadened systems. Study of the influence of semiconductor laser design on information transmission. Investigation of the ability to use scattered light to detect the presence of encapsulated aerosols. This work involves decision theory, and both inverse scattering and pattern recognition problems.

CLARK ATLANTA UNIVERSITY
223 James P. Brawley Dr.
Atlanta, GA 30314

298. CHARACTERIZATION OF HYDROGEN COMPLEX FORMATION IN III-V SEMICONDUCTORS

M. Williams, Department of Physics
(404) 880-6902 02-2 $99,172

Investigations are performed on the formation, properties and stability of hydrogen complexes in InP, As and P based ternary and As-P based quarternary semiconducting materials. The diffusion depths for atomic hydrogen for the various materials is being studied. The effects of this process on the electronic structure of the materials is also being investigated.

CLEMSON UNIVERSITY
Clemson, SC 29634-1911

299. CHARACTERIZATION AND THERMOPHYSICAL PROPERTIES OF BI-BASED SUPERCONDUCTORS: PART B

G.X. Tessema, Department of Physics and Astronomy
(864) 656-4350 01-3 $68,000

This involves a systematic substitution of Cu in CuO layers of the 2212 and 2223 phases of high temperature superconductors by transition metals (Fe, Co, Ni, Zn). The issue of whether the superconducting pairing state of the cuprates has d-wave or s-wave orbital symmentry can be addressed by studying the physical properties such as susceptibility, specific heat and transport.

COLORADO SCHOOL OF MINES
1500 Illinois St.
Golden, CO 80401

300. A NEW APPROACH TO VIBRATIONAL SPECTROSCOPY FOR THE CHARACTERIZATION OF BURIED INTERFACES

T.E. Furtak, Physics Department
(303) 273-3843 01-5 $153,000

The mechanism of surface vibrational sum-frequency generation will be studied for the electrochemical environment in stages. The sum-frequency generation will first be studied for metals under controlled conditions; then the vibrational sum-frequency generation from adsorbates on the metal surfaces will be examined. In parallel with the technique development, application will be made to the study of the ammonia fuel cell reaction. Identification of adsorbed intermediates will enable the determination between competing models for the mechanism of the oxidation. Thereafter, surface effects and alloy catalysts will be studied.

301. FRACTURE AND DEFORMATION OF CERAMIC/METAL JOINTS WITH GRADED MICROSTRUCTURES

I.E. Reimanis, Department of Metallurgical and Materials Engineering
(303) 273-3549 01-5 $99,960

The joining of dissimilar materials, specifically that of metal/ceramic joints is addressed for the case of graded microstructures. The goals include the experimental development of failure criteria for graded joints and advances in modeling and understanding of graded microstructures.

COLUMBIA UNIVERSITY
1106 Mudd Building
New York, NY 10027

302. ISOTHERMAL NUCLEATION KINETICS OF SOLIDS IN SUPERCOOLED LIQUID SI

J.S. Im, Department of Metallurgy and Materials Science
(212) 854-8341 01-3 $93,962

Experimental verification of Classical Nucleation Theory; laser melting and quenching, thin Si films on SiO_2, photolithography-isolated and SiO_2 encapsulation of Si films, supercooling, *in situ* detection of liquid-to-solid transformation via reflectivity measurements; isothermal nucleation and nucleation rates; tests of Turnbull's empirical generalization of proportionality between surface energy and heat of fusion and of Spaepen's theoretical prediction of temperature dependence of the liquid-solid interfacial energy.

303. PROTONS AND LATTICE DEFECTS IN PEROVSKITE-RELATED OXIDES

A.S. Nowick, Henry Krumb School of Mines
(212) 854-2921 01-3 $108,107

Defect chemistry of pure and doped perovskite-related oxides such as $BaCeO_3$, using internal friction, EPR, and IR techniques, together with electrical conductivity and dielectric relaxation measurements. Computer simulation techniques to study and predict defect-dopant behavior. Study of the Jonscher "universal" relaxation effect in crystalline ceramics and glasses over a wide temperature range.

CORNELL UNIVERSITY
120 Day Hall
Ithaca, NY 14853-2501

304. DISORDER AND NONLINEARITY IN MATERIAL SCIENCE: MARTENSITIC, CRACKS AND HYSTERESIS

J. A. Krumhansl, Department of Physics
(607) 255-5132

J. P. Sethna, Department of Physics 01-1 $80,880

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

305. UHV-STEM STUDIES OF MATERIALS

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

E. J. Kirkland, School of Applied and Engineering Physics
(607) 255-3332 01-1 $113,410

Extension of the present capabilities of quantitative microscopy with atomic resolution and application to determine the electronic, chemical and geometric structures such as quantum wells, grain boundaries and other defects. Nanodiffraction, X-ray spectroscopy, EELS and annular dark field imaging will be used to study imperfections in a variety of model systems including iron-silicon, titanium-aluminum, Ni_3Al as well as layered systems of copper-cobalt, iron-cobalt and iron-germanium.

306. DEFECTS AND TRANSPORT IN MIXED OXIDES AND THE KINETICS OF SOLID STATE REACTIONS

R. Dieckmann, Department of Materials Science and Engineering
(607) 255-4315 01-3 $97,900

Systematic thermogravimetric and coulombic titration studies of iron-based oxide solid solutions with rock salt and spinel structure to determine defect concentration. Thermogravimetric work on the influence of boundaries on the oxygen content of polycrystalline, nonstoichiometric oxides. Radioactive cation tracer diffusion work on a variety of mixed oxides. Electrical conductivity studies of ternary and quaternary systems, beginning with the system Co-Fe-Mn-0 to understand influence of space charges on observed electrical conductivity minimum.

307. QUASICRYSTALS GEOMETRICS AND ENERGIES

C. L. Henley, Laboratory of Atomic and Solid State Physics
(607) 255-5056 02-3 $60,450

The understanding of energetics governing the structure of quasicrystalmaterials from the microscopic level (effective interatomic potentials),to the tiling level (Hamiltonian for energy differences among tilings) andon to the macroscopic level (elastic theory). Particular emphasis placedon the i(AlCuLi) family of quasicrystals and also on hypotheticalboron-based structures. Investigation of geometrical properties ofmodels, particularly as defined various models. Development of computational methods for random-tiling simulations. Study (rigorously) how minimizing a tile Hamiltonian or optimizing spherepacking can enforce a ground state build from larger tiles.

308. CLUSTER AND LAYERED CHALCOGENIDES

F. J. DiSalvo, Department of Chemistry
(607) 255-7238 03-1 $146,000

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 will 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, superconducting and magnetic behavior and thermally induced valence transitions of post-transition elements to be determined. Study of Mo_3X_3 infinite chain clusters and polymer blends of these inorganic polymers with organic polymers. Synthesis of complexes of Nb_6I_8 with bifunctional ligands or with square planar metalorganic 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

309. THE YIELD STRENGTH ANOMALY AND ENVIRONMENTAL EFFECT IN FEAL

I. Baker, Thayer School of Engineering
(603) 646-2184 01-2 $87,125

Mechanical behavior of B2 intermetallics, particularly FeAl. Relationship between grain boundary structure/chemistry and the occurrence of intergranular fracture of FeAl and NiAl. Grain boundary characterization using AES and EDS/EELS on a FEG STEM. Compositional and temperature dependence of the flow and fracture of FeAl. Effect of boron on the strength of FeAl as a function of aluminum concentration and temperature. Effects of grain size and of boron on the strain-rate sensitivity of the room temperature fracture behavior.

310. EXCITONS AND PLASMAS IN SEMICONDUCTING MICROSTRUCTURES

M. Sturge, Department of Physics
(603) 646-2528 02-2 $100,000

Spectroscopic investigations on three types of semiconductor systems: Type II indirect gap superlattices, strain confined quantum structures and partially ordered ternary semiconductors to improve the understanding of optically excited states of such structures. Time-resolved tunable laser spectroscopy, magneto-spectroscopy and spatially resolved spectroscopy, with and without external perturbations such as magnetic field, electric field and uniaxial stress, will be employed as experimental tools.

UNIVERSITY OF DELAWARE
Newark, DE 19716

311. FUNDAMENTAL STUDIES OF NOVEL PERMANENT MAGNET MATERIALS

G. C. Hadjipanayis, Department of Physics
(302) 831-2661 02-2 $0 (0 months)

Research to advance the understanding of the magnetic rare earth - transition metal compounds and alloys that have high Curie temperatures and large magnetization. The materials studied usually are based on iron and light rare earths, and are generally ternary or higher order alloys with unusually complex, anisotropic structures. Investigated are Fe-rich phases which have been nitrogenated or carbonated to enhance their magnetic properties, new phases reached by intermediate metastable phases via melt spinning, materials produced by mechanical alloying in a high energy ball mill under inert atmosphere, and nanostructured and nanocomposite films made by sputtering techniques. Extensive characterization of the materials by comprehensive experiments which include X-ray and neutron diffraction, electron microscopy, dc and ac magnetic susceptibility, Fe^{57} Mossbauer, and photoemission. Spin-polarized, self-consistent electronic structure calculations performed to compare with the experimental results. Research performed in close collaboration with work at the University of Delaware.

DUKE UNIVERSITY
Box 90291
Durham, NC 27708-0291

312. GROWTH AND CHARACTERIZATION OF MBE PARAMETRIC VARIATIONS UPON POLARIZATION INDEPENDENT STRAINED FILMS

T. Daniels-Race, Department of Electrical and Computer Engineering
(919) 660-5258 02-2 $101,463

The effect of molecular beam epitaxy (MBE) controlled growth kinetics on strained thin films which exhibit novel reactions to polarized light is investigated. Objectives include the elucidation of the effects of MBE controlled and structurally based parameters upon strain phenomena, the growth of high quality tensile strained heterolayers in materials systems amenable to GaAs and InGaAs substrate processing chemistry, and the effects of strain upon energy band transitions.

FISK UNIVERSITY
Nashville, TN 37208

313. METAL COLLOIDS AND SEMICONDUCTOR QUANTUM DOTS: LINEAR AND NONLINEAR OPTICAL PROPERTIES

D.O. Henderson, Physics Department
(615) 329-8622 01-3 $101,629

Synthesis of nanocomposite materials consisting of metal colloids and semiconductor (II-IV and III-V) quantum dots by ion implantation. Laser and thermal post-processing to control and modify optical characteristics. Spectroscopic examination of optical properties and host-guest interactions. Size and morphology information of colloids via TEM and AFM examination. Relationship between materials and fabrication routes on nonlinear optical response.

FLORIDA STATE UNIVERSITY
1800 East Paul Dirac Dr.
Tallahassee, FL 32306

314. CORRELATED ELECTRONS IN REDUCED DIMENSIONS

N. E. Bonesteel, Department of Physics and NHMFL
(904) 644-7805 02-3 $42,715

Theoretical studies of electron systems in two and one dimensional quantum confined structures. Numerical simulations of incompressible fractional quantum Hall States. Investigation of the physical consequences of the Halperin-Lee-Read gauge theory of gamma=1/2 composite fermion metal in double layer quantum phase transitions. Investigation of electron correlations in a quantum wire.

315. INVESTIGATIONS OF THE DYNAMICS AND GROWTH OF SURFACES AND ULTRATHIN FILMS BY HELIUM ATOM SCATTERING

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

S. A. Safron, Department of Chemistry
(904) 644-5239 02-4 $59,000 (6 months)

High-resolution helium atom scattering will be used to investigate the microscopic interactions controlling epitaxial growth and the formation of overlayers, the surface structure, lattice dynamics and phase changes in ionic metal oxides, and energy exchange in multiphonon surface scattering.

UNIVERSITY OF FLORIDA
Gainesville, FL 32611-2085

316. QUANTUM-CONFINEMENT EFFECTS AND OPTICAL BEHAVIOR OF INTERMEDIATE SIZE SEMICONDUCTOR CLUSTERS IN GLASS

J.H. Simmons, Department of Materials Science and Engineering
(904) 392-6679

P. H. Kumar, Department of Physics
(904) 392-6679 01-1 $115,286

Studies performed on the quantum confinement effects and optical behavior of semiconductor clusters in glass.

Preparation and study of CdTe, Si, Ge, GaAs, and GaN clusters in silica, titanium silicate, ITO (indium-tin-oxide), and several heavy metal oxides including In_2O_3, and a complex glass developed by the PI, $PbO-B_2O_3-Ga_2O_3-In_2O_3$. Structural studies will include TEM and photoemission. Optical behavior to be afforded by absorption spectroscopy, Raman, transient absorption, and photoluminescence. Loading studies will determine the effect of tunneling. Carrier diffusion and conductivity to be determined as well as Hail Effect in conducting matrices. Studies of the nature and energy of quantum states which originate from bands other than at the gamma point.

317. INSTRUMENTATION FOR THE MRCAT UNDULATOR BEAMLINE AT THE ADVANCED PHOTON SOURCE

R. S. Duran, Department of Chemistry
(352) 392-2011 02-2 $267,560

Completion of an undulator beamline and associated experimental facilities at Sector 10 of the Advanced Photon Source by the Materials Research Collaborating Access Team (MRCAT). Experiments involving high resolution in space, momentum and time-studies of catalysts, polymers, organic monolayers, liquid-solid and solid-solid interfaces, fuel cells, and thin liquid films.

318. SCATTERING STUDIES OF ORDERING PROCESSES AND QUANTUM EXCITATIONS

S. E. Nagler, Department of Physics
(904) 392-8842 02-2 $51,001

X-ray and neutron scattering are being used to investigate ordering processes and the microscopic structure of materials undergoing phase separation or ordering. Systems under investigation include the quantum binary alloy, solid $^3He/^4He$, undergoing phase separation and free-standing soap films undergoing a thinning process constituting an ordering mesoscopic system in a confined geometry.

319. STUDIES OF HIGHLY CORRELATED ELECTRON MATERIALS: SUPERCONDUCTIVITY

G. R. Stewart, Department of Physics
(904) 392-9263/0521 02-2 $90,000

Experimental investigations will be made on highly correlated electron "heavy fermion" materials to understand what parameters control the nature of the normal and/or superconducting ground state formed. Focus will be on further hydrogen doping; extending the scope of specific heat-resistivity correlations; fully characterizing ultra-pure UBe_{13} samples already produced; supercondctivity suppression due to ligand doping of UBe_{13} with magnetic ions. Complementary cerium based work will be continued. Compounds will be obtained or prepared and characterized by X-ray and neutron diffraction, resistivity, dc and ac susceptibility, and specific heat (often with applied magnetic field) measurements.

320. TIME-RESOLVED FAR-INFRARED EXPERIMENTS AT THE NSLS

D. Tanner, Physics Department
(904) 376-0614 02-2 $108,353

A facility for time resolved infrared and far-infrared spectroscopy will be built on Beamline U12(IR) at the National Synchrotron Light Source. Time resolution is achieved through pump-probe techniques so that existing detection technologies can be utilized. This will enable studies of dynamics in semiconductors and superconductors and on surfaces.

321. NANO-MACHINING VIA ION-SURFACE INTERACTIONS

H.-P. Cheng, Department of Physics and Quantum Theory Project
(352) 392-6256 02-3 $40,000

The object of the proposal is to study controlled surface modifications by ion-surface interactions, a set of topics collectively called nano-machining. The investigation includes the dynamics of Coulomb explosions, charge transfer processes, defect formation, shockwave propagation, energy dissipation, desorption, and sputtering yields. Large-scale molecular dynamics (MD) simulations will be employed in a generalized electronic-atomic framework.

GEORGE MASON UNIVERSITY
4400 University Drive
Fairfax, VA 22030-4444

322. THEORETICAL STUDY OF PHONON MODES AND ELECTRON-PHONON SCATTERING IN STRUCTURALLY MODIFIED ELECTRONIC MATERIALS

C. McIntyre, Department of Physics & Astronomy
(703) 993-1286 02-2 $100,000

The effects of multilayers crystalline materials on phonon modes and electron-phonon interactions are being investigated. Emphasis is on characterizing the phonon modes of sharp interfaces and analyzing the role of interfacial disorder on the phonon spectrum and electron-phonon interaction. Structurally modified materials, including quantum wells and superlattices with semiconductor components, are covered by the investigation.

GEORGIA INSTITUTE OF TECHNOLOGY
Atlanta, GA 30332-0430

323. FIRST-PRINCIPLES STUDY OF HYDROGEN IN SOLIDS AND ON SURFACES

M. -Y. Chou, Physics Department
(404) 894-4688   02-2 $70,000 (10 months)

Problems to be investigated include: disorder-disorder, disorder-order and order-order phase transitions found in temperature-composition diagrams; preferential interstitial sites of hydrogen in different metals and in metal thin films, the change of optimal sites under pressure or uniaxial stress; the vibrational spectra, diffusion 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.

324. EPITAXIAL PHENOMENA

A. Zangwill
(404) 894-7333   02-3 $65,000

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

325. ASSESSING THE IMPACT IN INDUSTRY OF BASIC RESEARCH SPONSORED BY THE OFFICE OF BASIC ENERGY SCIENCES - AN "R&D VALUE MAPPING" APPROACH

J. B. Bozeman
(404) 894-3196

D. Roessner
(404) 894-0093   03-3 $186,891

The impact on industry of public investment in basic research is being evaluated. A modified case study design, "R&D Value Mapping," will be employed, seeking to identify the impacts and benefits that industry experiences subsequent to interacting with basic research projects supported by DOE's Office of Basic Energy Sciences. It is intended that these industry impacts be linked to a series of upstream factors that can be influenced by DOE program managers, such as project funding mix and choice of mechanism for industry interaction.

GEORGIA TECH RESEARCH CORPORATION
Atlanta, GA 30332-0430

326. STRUCTURE AND DYNAMICS OF MATERIAL SURFACES, INTERPHASE-INTERFACES AND FINITE AGGREGATES

U. Landman, School of Physics
(404) 894-3368   02-3 $290,000

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

327. THE ORGANIC CHEMISTRY OF CONDUCTING POLYMERS

L. M. Tolbert, Department of Chemistry
(404) 894-4043   03-1 $75,000

The phenomena of charge transport in conducting polymers, materials which are ordinarily insulators, is basically a problem in mechanistic organic chemistry. Fundamental studies in the mechanistic organic chemistry of conducting polymers are being conducted. Oligomers of defined length have been synthesized, and a comparison of their spectroscopic properties as they converge with those of the associated polymers is being carried out. This approach has allowed a validation of solid state theory for these materials. 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.

HARVARD UNIVERSITY
29 Oxford Street
Cambridge, MA 02138

328. CRYSTAL GROWTH KINETICS AT EXTREME DEVIATIONS FROM EQUILIBRIUM
M. J. Aziz, Division of Applied Science
(617) 495-9884 01-1 $79,023

Fundamental study of materials growth during Pulsed Laser Deposition. Ballistic aspects of impingement and deposition. Effects of surface relaxation, roughening, adsorption and incorporation.

329. FUNDAMENTAL PROPERTIES OF LIGHT ATOMS AND SPIN-POLARIZED QUANTUM SYSTEMS
I. F. Silvera, Lyman Laboratory of Physics
(617) 495-9075 02-2 $150,000

Investigation of light bosonic atoms at low temperature and high density to observe the effects of quantum degeneracy in condensed systems of identical particles. Attempt to reach sufficient densities and low temperatures that these unusual gases will undergo Bose-Einstein condensation using either a hybrid trap consisting of a static magnetic trap and a microwave trap or the formation of a two-dimensional gas of spin polarized hydrogen on a helium surface in a magnetic field gradient. nvestigation of helium at microkelvin temperatures by evaporation of helium films from low temperature surfaces to achieve extremely low temperatures and high densities so that quantum degenerate effects and the possible formation of extremely weakly bound helium dimers in equilbrium with the gas can be studied.

330. SYNCHROTRON STUDIES OF LIQUID METAL SURFACES
P. S. Pershan, Division of Applied Sciences
(617) 495-3214 03-3 $80,000

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

UNIVERSITY OF HOUSTON
Houston, TX 77204-4792

331. THE ROLE OF CRACK FACE BRIDGING MECHANISMS IN THE FATIGUE RESISTANCE OF NON-TRANSFORMING CERAMICS
K.W. White, Department of Mechanical Engineering
(713) 743-4526 01-2 $75,460

Determination of microstructural role of crack face bridging mechanisms in non-transforming ceramics subjected to cyclic loading environments. Application of post-fracture tensile experiments to evaluation of the wake process zone resulting from static crack extension with the goal of obtaining improved resolution of the mechanistic constitutents and the resolution of the separate components of the fracture process. Correlation of the components of the fracture process with the character of the microstructural constituents. Fatigue crack growth experiments to temperatures of 1200°C so as to permit the delineation of the thermoelastic contributions at the lower temperatures which may dominate the behavior at lower temperatures and other mechanisms involving interphases and interfaces which may dominate the behavior at higher temperatures.

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

Operation of a dedicated glass and liquid neutron diffractometer (GLAD) at the Intense Pulsed Neutron Source (IPNS) of Argonne National Laboratory with collabortive support from Argonne personnel. Determination of the atomic structure of glasses and/or amorphous materials by the utilization of X-ray and neutron scattering methods closely coupled with model computer calculations. Examples of materials investigated are sputtered IrO_2 films, molten $FeCl_3$, amorphized silicon and its annealing behavior, and nanophases of zeolites and related molecular sieves. Some studies of laser light scattering from colloidal and polymeric systems.

HOWARD UNIVERSITY
Washington, DC 20059

333. ENGINEERING, DESIGN, AND CONSTRUCTION OF THE MHATT-CAT SECTOR AT THE ADVANCED PHOTON SOURCE

W. Lowe, Department of Physics and Astronomy
(202) 806-4351 02-2 $2,300,000 (11 months)

Design, construction and operation of the University of Michigan, Howard University and AT&T Bell Laboratories Collaborative Access Team (MHATT-CAT) beamlines at the Advanced Photon Source will be performed. Research includes time-resolved studies of materials under dynamic conditions: the microscopics of physical and chemical processing, behavior under stress and structural relaxation and the kinetic mechanisms of growth.

UNIVERSITY OF ILLINOIS AT CHICAGO
845 W. Taylor Street
Chicago, IL 60607-7059

334. MATERIALS PROPERTIES AT INTERNAL INTERFACES: FUNDAMENTAL ATOMIC ISSUES

N. Browning, Department of Physics
(312) 413-8164 01-6 $206,140 from prior year

Experimental study of interfaces at atomic resolution using a scanning transmission electron microscopy. Direct location of cations by the Z-contrast technique and composition and bonding information from electron energy loss spectroscopy (EELS). Use of EELS and the development of energy loss near-edge structure (ELNES) for a study of cation location, bonding and its nearest neighbors in a series of undoped and donor/acceptor doped $SrTiO_3$ grain boundaries.

UNIVERSITY OF ILLINOIS
104 South Wright Street
Urbana, IL 6180

335. OXIDE FILM MICROSTRUCTURE: THE LINK BETWEEN SURFACE PREPARATION PROCESSES AND STRENGTH/DURABILITY OF ADHESIVELY BONDED ALUMINUM

K.J. Hsia, Department of Theoretical and Applied Mechanics
(217) 333-2321 01-5 $607,270 from prior year

Experiment, modeling, and testing of relationship between surface preparation and strength/durability prediction in the bonding of aluminum and its alloys for automobile applications. Process development to synthesize improved surface preparation techniques. Identification of microstructural parameters that determine bond strength including porosity, pore connectivity, pore size distribution, and protrusion morphology. Mechanistic development between processing and microstructure, and between microstructure and bond strength and durability. Employment of surface analytical techniques and mechanical testing. Development of quantitative models of thin film growth.

INDIANA UNIVERSITY
Bloomington, IN 47405

336. NEUTRON POLARIZERS BASED ON POLARIZED ^{3}HE

W. M. Snow, Department of Physics
(812) 855-7914 02-1 $0 (0 months)

Develop neutron polarizer based on an absorbing gas of polarized ^{3}He atoms. The ^{3}He gas is to be polarized either by spin-exchange with polarized alkali atoms or by optical pumping.

JOHNS HOPKINS UNIVERSITY
Baltimore, MD 21218

337. IN SEARCH OF THEORETICALLY-PREDICTED MAGIC CLUSTERS: TOWARD THE DEVELOPMENT OF A NEW CLASS OF MATERIALS
K.H. Bowen, Department of Chemistry
(410) 516-8425 01-1 $127,037

Systematic experimental search for theoretically-predicted magic clusters. Formation of magic clusters by several methods. Detection by mass spectrometry. Synthesis of macroscopic samples of clusters.

338. INTERFACE ENERGIES AND THE STABILITY OF MULTILAYER MATERIALS
T.P. Weihs, Department of Materials Science and Engineering
(410) 516-4071 01-2 $81,186 (8 months)

Free energies of solid-solid interfaces: grain boundaries and between alternate layers. Fabrication of chemically stable multilayered foils. Structural stability of multilayered materials.

KANSAS STATE UNIVERSITY
116 Cardwell Hall
Manhattan, KS 66506

339. OPTICAL AND ELECTRICAL PROPERTIES OF III - V NITRIDE WIDE BANDGAP SEMICONDUCTORS
H. Jiang, Department of Physics
(913) 532-1627 02-2 $50,000

Optical and electrical properties of GaN and $Al_xGa_{1-x}N$ will be studied including alloys, epitaxial layers, and quantum well structures. The recombination rates for all possible mechanisms will be studied by time-resolved picosecond laser spectroscopy. These will be characterized as a function of temperature, alloy composition, applied electric and magnetic fields, and parameters of the exciting photons. Non-linear properties will also be measured. Electrical property measurements will focus on the effects of p-type dopants and native defects at temperatures up to 600 degrees Centigrad.

340. STRUCTURE, DYNAMICS AND THERMODYNAMICS OF METAL SURFACES
T. S. Rahman, Department of Physics
(913) 532-1611 02-3 $40,633

The theoretical study will investigate the temperature dependent microscopic structure, dynamics, and thermodynamical properties of stepped transition metal surfaces. Many body potentials will be used to study a set a vicinal surfaces including the metals, Al, Cu, Ag, and Pt. The effect of atomic vibrations will also be included.

UNIVERSITY OF KENTUCKY
Lexington, KY 40506-0055

341. DYNAMIC FLUX LINE RESPONSE IN LAYERED SUPERCONDUCTORS WITH TAILORED DEFECT STRUCTURES
L. DeLong, Department of Physics & Astronomy
(606) 257-4775 02-2 $50,000 (2 months)

Electron beam lithography is to be used to provide controlled columnar defects in high quality Pb/Ge and WGe/Ge multilayer materials. These will be studied using vibrating reed and torque magnetometry and ac susceptibility. These artificial structures are models for layered superconductors, such as the high-T_c cuprates, with columnar defects. Because of the extensive capability to control nearly all parameters in these model systems, they provide unique opportunities to test both fundamental many-body theories and quantitative models of magnetic flux line dynamics in irradiated high-T_c materials.

342. SOLID STATE ELECTRONIC STRUCTURE AND PROPERTIES OF NEUTRAL CARBON-BASED RADICALS
R. C. Haddon, Departments of Chemistry and Physics
(606) 257-8844 03-1 $70,998 (10 months)

This research is directed towards the synthesis of organic solids derived from neutral radicals which are derivatives of the phenalenyl system. Many compounds in this series should be solid state organic conductors. Some may be metallic and may possibly be superconductors. The solid state properties of these systems in the context of their electron transport and magnetic properties are main issues. The virtue of these systems is that they are overall neutral and can be sublimed and transferred into films. A long term thrust of this work is to understand the relationship between solid state properties and molecular structure.

343. KY DOE/EPSCOR PROGRAM
J. M. Stencel,
(606) 257-0250 05-1 $750,000

The DOE/EPSCoR program in Kentucky will enhance the State's research competitiveness in the energy-related areas of fossil energy, studies of organic carbon in reservoir systems, high energy and nuclear physics, and materials research. The work of the fossil energy research team, primarily intended to abate pollution, includes the creation of a pulsed-neutron-based on-line coal characterization system, coal cleaning studies, and the development of a continuum mechanics model to aid in the mixing of silo coals. As quality of life and the enhanced economic growth of Kentucky and the Nation are directly tied to its water resources, the reservoir characterization team is conducting studies to understand the effect on water quality caused by the transport, accumulation, and use of organic carbon in large reservoir systems. Kentucky's high energy and nuclear physics programs are helping advance the state of knowledge in these two important fields. The high energy research group is conducting lattice gauge calculations on massively-parrallel computers to study the structure and interaction of nucleons and the heavy-light mesons. The nuclear physics research team is helping advance the spin physics program at the Thomas Jefferson National Accelerator Faculty by designing and building a moller Polarimeter and by initiating work in beam polarimetry and polarized targets. The preparation of ZrO_2 for thermal barrier coatings is the focus of Kentucky's fourth research cluster. These coatings have important applications in areas like turbine blade lifetime enhancement.

LEHIGH UNIVERSITY
5 East Packer Avenue
Bethlehem, PA 18015

344. DETERMINATION OF STRUCTURE AROUND LIGHT ATOMS IN INORGANIC GLASSES BY EXELFS
H. Jain, Department of Materials Science and Engineering
(610) 758-4217 01-1 $119,194

Structure of inorganic glasses, especially short range order around glass modifier alkali ions and the network forming oxygen atoms. An experimental study of the validity of the modified network model (MRN), using extended energy loss fine structure (EXELFS) with energy-filtered electron diffraction. The local structure around both alkali and oxygen ions, measured by this technique, will be used with simulation studies to establish fundamental glass structure, and, in turn, physical properties of glasses.

LOUISIANA BOARD OF REGENTS
2000 Percival Stern Hall
New Orleans, LA 10118

345. DOE EPSCOR PROPOSAL FOR THE STATE OF LOUISIANA
C. F. Ide,
(504) 865-5546 05-1 $658,816

Louisiana will carry out DOE/EPSCoR research activities in two areas: "Inorganic Synthesis and Laser-Induced Photochemistry Relevant to the Fabrication of Electronic Materials" focuses on electronic materials research which includes the synthesis of novel materials precursors, the application of unique thin-film deposition strategies, and the utilization of innovative photochemical techniques. "Development of Mammalian and Non-Mammalian Toxicological Indices to Investigate Risks Associated with Energy-Related Wastes" focuses on the toxicological consequences of exposure to energy-related materials and wastes at several levels, including: ecosystems, populations, organisms, specific tissues and molecular level interaction, with emphasis on the genetic, reproductive risks and trophic relationships. Assessments of the impacts of exposure to contaminants on metabolic function of liver, gill, lung and central nervous systems will also be performed using several endpoints. In the area of human resource development, at the precollege level, Louisiana is proposing to: (1) continue the Research Internship f0r Precollege Science Teachers, which offers research experience with the DOE/EPSCoR cluster scientists; (2) disseminate approximately 500 copies of the science manuals developed for high school teachers through the Project ENERGIZE! program; and (3) develop synergistic efforts, i.e., information exchange for summer internships and other opportunities, joint conferences, seminars and workshops; technical support and participation in the Hands-on Universe project. For postsecondary activities, Louisiana will: (1) continue the mentoring program for high potenial undergraduates and the involvement of junior faculty and graduate students in energy-related research; (2) host a DOE/EPSCoR Science, Engineering and Math Research Conference in conjection with the National Science Foundation (NSF); and (3) provide for undergraduate students academic year and summer in-state research support, and summer research internships at national laboratories or energy-related industries each summer.

LOUISIANA STATE UNIVERSITY
Baton Rouge, LA 70803-4001

346. MOLECULAR DYNAMICS SIMULATIONS OF NANOSTRUCTURED MATERIALS ON PARALLEL COMPUTERS

P. Vashishta, Concurrent Computing Laboratory for Materials Simulations
(504) 388-1342

R. Kalla
(504) 388-1157

G. Greenwall
(504) 388-1342 02-3 $37,500

Large scale molecular dynamics simulations of ceramic and semiconductor systems are carried out at the microscopic level. Mechanical properties of environmentally banign sustances such as aerogel silica will be studied. As will be thermal properties of ceramic silicon nitrides, and the crack propagation and fracture of thin films of these materials. In addition new algorithms for parallel, distributed memory computing will be implemented.

MAINE SCIENCE & TECHNOLOGY FOUNDATION
87 Winthrop Street
Augusta, ME 04330

347. MAINE DOE/EPSCOR IMPLEMENTATION PROGRAM

T. Shehata,
(207) 621-6350 02-5 $600,000

Over the past years of the Maine EPSCoR program, major new research initiatives have been implemented with new faculty, new research programs and opportunities for Maine students at all education levels. The present grant supports research clusters (Human Genome Project: Technology for Studying Hierarchical Chromosome Organization and Research Cluster for Micro-Tribology: Friction and Wear in Advanced Materials) and several human research development activities.

UNIVERSITY OF MAINE
5764 Sawyer Research Ctr.
Orono, ME 04469

348. SYNTHESIS, CHARACTERIZATION AND MECHANICAL BEHAVIOR OF BINARY AND TERNARY OXIDE FILMS

R. J. Lad, Laboratory for Surface Science and Technology
(207) 581-2257 01-1 $71,923

Fundamental properties of metal/oxide and oxide/oxide heterogeneous interfaces with emphasis on effects of interfacial defects, impurities, carbon layers, and amorphous phases on interfacial morphology, adhesion, electronic structure, and high temperature stability. Deposition of ultra-thin metal and oxide films (viz. Al, Ti, Cu, Mg0, Y_2O_3, and SiO_2) on single crystal Al_20_3 substrates. Determination of film epitaxy and interface morphology by in-situ RHEED analysis and Atomic Force Microscopy; determination of composition, chemical bonding, interdiffusion, segregation and electronic structure information by X-ray and ultraviolet photoemission, Auger spectroscopy, and EELS.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
77 Massachusetts Avenue
Cambridge, MA 02139

349. THE PREDICTION OF PHASE STABILITY AND STRUCTURE IN COMPLEX OXIDES

G. Ceder, Department of Materials Science and Engineering
(617) 253-1581 01-1 $98,000

First-principles calculations on oxides. Prediction of structure and defect arrangements at non-zero temperature. Mechanisms of charge compensation in doped oxides. Phase diagrams. Diffusion in highly concentrated solid solutions. Current applications include doped zirconia for solid electrolytes and lithium-transition-metal oxides for rechargeable batteries. Computational tools include pseudopotential method, tight binding and LMTO. Ionic disorder is modeled with a generalized lattice model and Monte Carol sampling.

350. CERAMIC INTERFACES

Y-M. Chiang, Department of Materials Science and Engineering
(617) 253-6471 01-2 $95,230

Defect thermodynamics of interfaces in CeO_2 and TiO_2. Electrical characterization of nanocrystals and thin films. Space-charge experiments in polycrystals. Interfacial forces leading to destabilization of thin intergranular films in ceramics using measurements of pressure vs. film thickness and dihedral angle in ZnO-Bi_2O_3 and TiO_2-SiO_2. Impedence spectroscopy, HREM, and STEM.

351. THERMO-MECHANICAL RESPONSE OF LAYERED MATERIALS

S. Suresh, Department of Materials Science and Engineering
(617) 253-3233 01-2 $108,326

The micromechanics of thermo-mechanical deformation and failure is addressed from a experimental and theoretical standpoint for both homogeneous and compositionally graded layers.

352. STRUCTURAL DISORDER AND TRANSPORT IN TERNARY OXIDES WITH THE PYROCHLORE STRUCTURE

H. L. Tuller, Department of Materials Science and Engineering
(617) 253-6890 01-3 $116,505

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. Computer simulations of defects, transport and structural parameters in these systems. Structural disorder characterized by X-ray diffraction, neutron diffraction, and spectroscopic measurements. Electrical and defect properties characterized by AC impedance, DC conductivity, thermoelectric power, and thermogravimetric techniques. Materials to be doped and studied include Gd_2O_3-ZrO_2-TiO_2, Y_2O_3-ZrO_2-TiO_2 and related systems.

353. PROCESSING OF SUPERCONDUCTING OXIDES IN ELEVATED MAGNETIC FIELDS

J. B. Vander Sande, Department of Materials Science and Engineering
(617) 253-6933 01-3 $117,635

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

354. RADIATION-INDUCED TOPOLOGICAL DISORDER IN IRRADIATED CERAMICS

L. W. Hobbs, Department of Ceramics and Materials Science
(617) 253-6835 01-4 $113,872

Fundamental study to characterize irradiation-induced amorphization of SiC, Si_3N_4 and $AlPO_4$. Irradiations to be performed in-situ with electrons in a TEM, with heavy ions using the implantation facilities, or with neutrons using available neutron sources. Energy-filtered electron diffraction (EFED) technique to examine the structure of topologically disordered ceramics; the use of X-rays, neutron and electron diffraction to study structure; proton and other ion irradiations to modify structures, and a new modelling program applying methods developed for self-assembly of virus shells from proteins to explore the process of topological disordering. Studies of neutron-irradiated single crystals of $Pb_2P_2O_7$ and high pressure polymorphs of silica will be completed.

355. DESIGN OF SURFACE TEXTURE FOR IMPROVED CONTROL OF FRICTION AND FORMABILITY OF ALUMINUM SHEET PRODUCTS FOR AUTOMOTIVE APPLICATIONS

L. Anand,
(617) 253-1635 01-5 $450,000 from prior year

The development of a more complete process design capability for a variety of sheet forming operations will be accomplished. To do this a set of constitutive equations for the mechanical and theoretical behavior of tool-workpiece interfaces will be developed. Computational procedures will also be developed to help automate this capability. Microscale sheet of surface geometry design will be optimized to reduce tool-surface friction and enhance formability.

356. GELS FOR MOLECULAR RECOGNITION, ACCUMULATION AND RELEASE

T. Tanaka,
(617) 253-4817 01-5 $375,000 from prior year

This project will expand the development of polymer gels that can selectively recognize, accumulate and release molecules. The essence of the design is that the polymer will consist of two groups of monomers, each with specific designated roles. One group will form a complex with a target molecule and the other group will allow the polymer gel network to reversibly stretch and shrink in response to planned environmental changes. The complexing sites will develop strong affinity to target molecules only when the gel is shrunken and the sites come into proximity with the target molecules. However, when the gel expands and stretches, the affinity for the target molecules is diminished. Thus, the affinity of the synthetic polymer gel network can be specifically controlled using reversible phase transition of the gel.

357. DEVELOPMENT OF BEAMLINES FOR CONDENSED MATTER PHYSICS AND MATERIALS SCIENCE AT THE ADVANCED PHOTON SOURCE

S. Mochrie,
(617) 253-6588 02-2 $490,000

Design, development and construction of the IMM-Collaborative Access Team (IMM-CAT) Beamline at the Advanced Photon Source for research on the structure and properties of advanced materials.

358. PHASE TRANSITION PHENOMENA IN QUENCHED DISORDERED AND QUANTUM-CORRELATED SYSTEMS

A. N. Berker, Department of Physics
(617) 253-2176 02-3 $52,866

Renormalization-group calculations will be performed for various models all incorporating some aspect of randomness. Possible novel hyperuniversality of critical phenomena where there is strong randomness will be investigated as a possible replacement for the ordinary universality -- shown previously to be violated in these systems. The tricritical point involving a conversion of first order phase transitions to second order by strong bond randomness will be investigated. Finite-temperature renormalization group theory will be applied to tJ and enhanced tJ models of electronic conduction in 1-3 dimensions. The hard-spin mean-field theory, previously applied to uniformly frustrated systems, will be applied to spin glasses. A speculative effort will the development of a non-equilibrium renormalization group theory based on the restriction by time scales of the underlying partial trace of the partition function.

359. SANS STUDIES OF INTERFACIAL CURVATURES IN BICONTINUOUS MICROEMULSIONS AND VISCOELASTICITY IN DENSE MICELLAR SOLUTIONS AND MICROEMULSIONS

S.-H. Chen, Department of Nuclear Engineering
(617) 253-3810 03-2 $66,667 (8 months)

A bicontinuous microemulsion is a micro-phase-separated mixture of oil and water made stable macroscopically by addition of a surfactant. Since the interfacial tension between oil and water is ultra-low because of thepresence of the surfactant, the curvature energies of the interface control the phase behavior. This program continues to develop Small Angle Neutron Scattering (SANS) methods based on contrast variations for direct measurements of curvatures of the oil-water interface in bicontinuous one-phase microemulsions. The aim is to measure the average mean curvature, the average mean square curvature, and the average Gaussian curvature of the oil-water interface in one-phase microemulsions as functions of temperature and surfactant volume fraction across the one-phase channel. The method is based on the application of the random wave model of bicontinuous microemulsions, originally proposed by Berk, using a specific form of the spectral density function proposed recently during this program. This method will be extended to non-isometric microemulsions, micellar and protein solutionsbased on a new theory developed recently by Cohen et. al. The role of SANS is to determine the microstructure of the colloidal solution which is the necessary input to the calculation of the viscoelasticity.

UNIVERSITY OF MASSACHUSETTS
Amherst, MA 01003-4530

360. SEGMENTAL INTERPENETRATION AT POLYMER-POLYMER INTERFACES

T. P. Russell, Polymer Science
and Engineering Department
(413) 545-0433 03-2 $0

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, 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.

MIAMI (OHIO) UNIVERSITY
Oxford, OH 45056

361. MAGNETIC MICROSTRUCTURE PHYSICS
M. J. Pechan, Department of Physics
(513) 529-4518 02-2 $39,000

Investigation of magnetic multilayers and magnetic quantum dots using ferromagnetic resonance and magnetization measurements. Determine interrelation of magnetic properties and interactions with structual and transport properties.

MICHIGAN STATE UNIVERSITY
East Lansing, MI 48824

362. LOCAL ATOMIC STRUCTURE OF SEMICONDUCTOR ALLOYS USING PAIR DISTRIBUTION FUNCTION ANALYSIS
S.J.L. Billinge, Department of Physics and Astronomy
(517) 353-8697

M. F. Thorpe, Department of Physics and Astronomy
(517) 355-9279 01-1 $104,667

Structural characterization of semiconductor alloys, utilizing diffraction data from X-rays or neutrons out to very large wavevectors. Accurate Pair Distribution Functions (PDF) to 20A and beyond to reveal local structure of alloy directly. Chemical clustering, and PDF peak shift and broadening caused by internal strains to be studied. Theoretical modelling to incorporate internal strains and thermal broadening. Techniques to be applied to $Ga_xIn_{1-x}As$ and $Si_{1-x}Ge_x$.

363. DISORDER AND FAILURE: PLASTICITY, FLUX FLOW AND FATIGUE
P. M. Duxbury, Department of Physics and Astronomy
(517) 353-9179 01-3 $93,962

Development of generic models for electrical, dielectric, mechanical and superconducting failure; analytic expressions for size effect, failure distribution, and crossover from nucleation stage to catastrophic failure stage. Nucleation and evolution of damage in random microstructures. Use of numerical methods such as finite element, finite difference or Green's function methods; complemented by scaling concepts such as fractals, percolation, and universality. Prediction of asymmptotic scaling laws such as ultimate tensile strength, damage prior to instability and fractal dimension of fracture surfaces. Development of broad theoretical understanding of the yield point in random plastic materials, the onset of flux flow in superconductors, fatigue in random materials, and the transmission of stress in random central-force problems. Methods applied specifically to mechanical properties of epoxy matrices containing high aspect ratio nano-dispersed clay platelets and to high-cyclic fatigue of Al/SiC composites. Material specific calculations compared with on-going experiments.

UNIVERSITY OF MICHIGAN
3003 S. State Street
Ann Arbor, MI 48109-1274

364. PARTICLE-INDUCED AMORPHIZATION OF COMPLEX CERAMICS
R.C. Ewing, Department of Nuclear Engineering and Radiological Sciences
(313) 647-8529 01-1 $107,306

Investigation of irradiation effects on transition from crystalline to aperiodic state in naturally occurring materials (complex oxides, silicates and phosphates) and ion-irradiated ceramics; effects of structure and bonding, cascade energy, defect accumulation and temperature on the amorphization of complex ceramic materials; structural types include zircon (ABO_4), olivine, garnet, alumino silicates, pyrochlore. Techniques include X-ray diffraction, high-resolution transmission electron microscopy (HRTEM), extended X-ray absorption fine-structure (EXAFS), and near-edge spectroscopy.

365. OXIDE CERAMIC ALLOYS AND MICROLAMINATES
I-W. Chen, Department of Materials Science and Engineering
(313) 763-6661 01-2 $0 (0 months)

Solute-defect interactions and segregation; CeO_2, Y_2O_3 and ZrO_2 host oxides; solid solutions with oxides of divalent Mg Ca and Sr, trivalent Sc, Yb, Y, Gd and La, tetravalent Ti and Zr, and pentavalent Nb and Ta. Static grain growth, dynamic grain growth and related mechanical phenomena; mechanisms for solute drag, solute-defect interactions; static grain growth experiments, grain boundary mobility, compression tests, dislocation creep; construction of stress-strain constitutive relation incorporating grain growth; microstructural and microchemical characterization. Densification kinetics, microstructure development, grain boundary mobility; doped solid solutions; effect of solute drag on sintering of second phase ceramics; effect of initial porosity. Deformation and fracture of ceramic slips. Plasticity induced interface instabilities. Sintering and microstructure development of bimaterials and compositionally graded materials. Strength and fracture of compositionally graded materials. Strength and fracture of layered, graded, and multiply connected cellular composites.

366. UNDERSTANDING THE MECHANISMS CONTROLLING ENVIRONMENTALLY-ASSISTED INTERGRANULAR CRACKING OF NICKEL-BASE ALLOYS
G. S. Was, Department of Nuclear Engineering and Radiological Sciences
(313) 763-4675 01-2 $150,378

Mechanisms of intergranular cracking in nickel-base alloys at high temperature and in high purity water. Development of creep and IGSCC resistant microstructures. Role of carbon as carbides and in solution in high temperature primary water. Role of grain boundary misorientation on IGSCC. Hydrogen effects on deformation and IG cracking.

367. INTERFACIAL DEFECTS, MORPHOLOGY AND KINETICS
D. J. Srolovitz, Department of Materials Science and Engineering
(313) 936-1740 01-3 $112,546

Theoretical approaches which range from analytical techniques to finite element methods and atomistic simulations, to provide information in three important areas: grain boundary migration under two distinct driving forces, grain boundary curvature and elastic energy; dislocation stand-off from heterophase interfaces in order to understand the mechanical consequences of variable bonding at interfaces; and the compositional and morphological stability of multilayers, in order to be able to predict the morphology of heteroepitaxial multilayer films and design stable multilayer structures.

368. SYNCHROTRON STUDIES OF NARROW BAND MATERIALS
J. W. Allen, Department of Physics
(313) 763-1150 02-2 $0 (0 months)

This experimental program utilizes a combined photoemission/inverse photoemission study of narrow band materials --- where additional effects of the Coulomb interactions can be expected to have greater significance. The focus is to relate the obtained spectroscopic properties to results obtained when only small excitation energies are involved. This is the crucial issue in attempting to use X-ray measurements to help unravel the thermal and electrical properties of a solid. The narrow band materials studied are selected on the basis of being the most stringent tests of our theoretical understanding.

369. GROWTH AND PATTERNS
L.M. Sander, Department of Physics
(313) 764-4471 02-3 $55,000

Analytic and simulation studies of the formation of solid state structure far from equilibrium will be performed. The effects of strain on the epitaxial growth of these films will be investigated. The stability of dense radial patterns arising from electrochemical deposition will be studied. New methods will be developed to study non-equilibrium continuum processes such as catalysis and other non-equilibrium processes.

MIDWEST RESEARCH INSTITUTE
425 Volker Boulevard
Kansas City, MO 64110

370. DESIGN AND CONSTRUCTION OF MAIN GROUP ELEMENT-CONTAINING MOLECULES AND MOLECULE-DERIVED MATERIALS WITH UNUSUAL ELECTRONIC, OPTICAL, AND MAGNETIC PROPERTIES
B.N. Diel,
(816) 753-7600 01-5 $600,000 from prior year

New Source compounds for the Metal Organic Chemical Vapor Deposition (MOCVD) of thin films, especially those which incorporate group IIIA (boron family) and group VA (nitrogen family) elements, and which are known to have utility as sensors in the automobile industry, are being developed, characterized, and evaluated with regards to volatility, thermal lability and thin film forming tendencies. Where appropriate, doped films and wafers are being prepared and evaluated and prototype devices fabricated.

UNIVERSITY OF MINNESOTA
421 Washington Ave., SE
Minneapolis, MN 55455

371. CRYSTALLINE-AMORPHOUS INTERFACES AND AMORPHOUS FILMS IN GRAIN BOUNDARIES

C.B. Carter, Department of Chemical Engineering and Materials Science
(612) 625-8805 01-1 $129,781

Thin and thick glassy films prepared on selected Al_2O_3 and MgO single crystal surfaces and in bicrystal boundaries; pulsed laser deposition; hot-pressing of bicrystals; tilt and twist boundaries, bicrystal orientation, interface plane and surface faceting. Structure and chemical analysis with visible-light microscopy, SEM, AFM and TEM, including bright - and dark-field imaging, HREM, EDS and PEELS; comparison of grain boundaries and interfaces with and without noncrystalline layers; wetting and dewetting of glassy films on grain boundaries; crystallization of glassy boundaries and interfaces. Computer modeling of amorphous/crystalline interfaces in collaboration with ANL; lattice statics and molecular dynamics.

372. THIN FILM ADHESION OF PRECRACKED FINE LINES

W.W. Gerberich, Department of Chemical Engineering and Materials Science
(612) 625-8548 01-2 $66,336

The need to determine accurate values of adhesion for thin films is addressed, first through examination of a new testing technique, the "Precracked Fine Line Scratch Test" (PLST) and second through the extension of the PLST technique to the measurement of interfacial adhesion of ductile thin films.

373. THEORETICAL STUDY OF REACTIONS AT THE ELECTRODE-ELECTROLYTE INTERFACE

J. W. Halley, Department of Physics and Astronomy
(612) 624-0395 01-3 $87,368

Electron transfer and other reactions of importance to aqueous corrosion are studied by simulation and modeling. Molecular dynamics used to describe solvent dynamics and tight bonding and local density function methods to study the electronic structure of metallic and oxide passivated electrodes. The calculations of atomic and electronic dynamics are linked to yield insights into such corrosion relevant phenomena as electron transfer, defect diffusion, polaronic electronic conductivity and cracking. Phenomena of particular interest include ferrous-ferric and cuprous-cupric outer shell electron transfer, the passivation layer of titanium, chloride at interfaces, hydrolysis at oxide surfaces and dissolution of metals. The project is part of an ongoing collaboration with Argonne National Laboratory.

374. THEORY OF THE STRUCTURAL AND ELECTRONIC PROPERTIES OF SOLID STATE OXIDES

J. R. Chelikowsky, Department of Chemical Engineering and Materials Science
(612) 625-4837 02-3 $59,000

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 psudopotential calculations, semi-empirical valence force field techniques, and the establishment of empirical chemical "scaling" indices. The amorphization in oxides induced by high pressure will be studied using classical and quantum mechanical techniques.

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

375. THEORETICAL STUDIES ON THE ELECTRONIC STRUCTURES AND PROPERTIES OF COMPLEX CERAMIC CRYSTALS AND NOVEL MATERIALS

W-Y. Ching, Department of Physics
(816) 235-2503 01-1 $147,930

Theoretical program to study the electronic structure and properties of complex ceramic materials. Over the next three year period the following will be carried out:
1) study of spinel ceramics of the form AB_2O_4, 2) study of defect and grain boundary structures, 3) modeling of Si-based oxide, nitride, and oxynitride glasses and their

interfaces with ceramic crystals, and 4) study of magnetic properties of permanent magnets such as $Nd_3Fe_{29-x}T_x$ (T=Ti or Cr), 5) study of novel materials and new methods of computation.

UNIVERSITY OF MISSOURI AT ROLLA
Columbia, MO 65211

376. DEVELOPMENT OF FOCUSING MONOCHROMATORS FOR NEUTRON SCATTERING INSTRUMENTS
M. P. Popovici, Research Reactor Center
(573) 882-5314 02-1 $150,000

Development of both the theoretical guidance and instrumentation for focusing neutron beams based upon bent crystals. These focusing neutron optics will be integrated into specialized monochromators for use in neutron diffraction and scattering experimentation.

377. A REVOLUTIONARY ROTATABLE ELECTRON ENERGY ANALYZER FOR ADVANCED HIGH-RESOLUTION SPIN-POLARIZED PHOTOEMISSION STUDIES
G. D. Waddill, Physics Department
(573) 341-4797 02-2 $129,990

Development and construction of an experimental photoemission system based upon a large-radius, rotatable hemispherical electron energy analyzer and an electron spin analysis capability. To be installed at the advanced Light Source (ALS) at LBNL.

THE UNIVERSITY OF MONTANA
Missoula, MT 59812-1002

378. THE MONTANA ORGANIZATION FOR RESEARCH IN ENERGY (MORE) COLLABORATIVE RESEARCH AND HUMAN RESOURCES DEVELOPMENT PROGRAM
J. Bromenshenk,
(406) 243-5648 05-1 $750,000

The University of Montana is conducting DOE/EPSCoR research activities in two areas. "Petroleum Reservoir Characterization," will develop a reservoir characterization team able to train a new, wholly-integrated earth scientist. The research plan developed by the cluster is based on the idea that maximum understanding of reservoir behavior is gained through integration of (1) 3-dimensional seismic illumination, (2) geologic models, (3) mathematical models that accommodate variations of physical scale and relative emphasis of data, (4) petroleum engineering models, and (5) a 3-dimensional visualization of the integrated model set. "Wind Energy Development," is divided into two project areas. In on project, wind turbine blades are being developed and tested. A test site has been established, the first turbine flown, and experimental blades for fatigue wear out studies have been developed. In this work, the test site will be expanded to include a larger turbine with more representative loading to bring the blade structural studies closer to utility grade turbine structural details. In a second area, the economics and use of wind generated energy, the effects of utility regulatory changes, and wind development on Blackfeet Tribal lands are being studied. One offshoot of the early work on this project was the development of an avian study that has received national attention and additional DOE funding. The Project Area will continue to pursue the avain issue and will explore additonal aesthetics-related siting concerns and issues related to wind development on Tribal lands. The development of wind resources is closely tied to the economics of wind energy use and the utility regulatory process, and studies have been proposed in these areas, as well as the related innovative use of wind energy in combination with other renewables and storage, particularly at remote sites.

NATIONAL ACADEMY OF SCIENCES
2101 Constitution Ave. NW
Washington, DC 20418

379. GENERAL/CORE SUPPORT FOR MATERIALS RESEARCH
R.E. Schafrik, Commission on Engineering and Technical Systems
(202) 334-3505 01-5 $50,000

Support for the National Materials Advisory Board and its forums, workshops, and studies.

380. SUPPORT OF THE SOLID STATE SCIENCES COMMITTEE
D.F. Morgan, Board on Physics and Astronomy
(202) 334-3520 02-2 $65,000

Support for the activities of the Solid State Sciences Committee and the Solid State Sciences Committee Forum.

381. AN ASSESSMENT OF CONDENSED MATTER AND MATERIALS PHYSICS
D. C. Shapero,
(202) 334-3520 02-2 $50,000

Support for activities of the Solid State Sciences Committee to perform a study to identify major recent achievements in condensed matter and materials physics; to identify new opportunities, needs, and challenges facing the field; and to articulate to the general audience the important roles played by condensed matter and materials physics in modern society.

NATIONAL SCIENCE FOUNDATION
4201 Wilson Boulevard
Arlington, VA 22230

382. CHEMMATCARS: A SYNCHROTRON RESOURCE FOR CHEMISTRY AND MATERIALS RESEARCH AT THE ADVANCED PHOTON SOURCE
H. Blount, Analytical and Surface Chemistry
(703) 306-1841 03-2 $350,000

Build and operate an undulator beamline at the Advanced Photon Source (APS) to perform structural and dynamic studies on liquid and polymer surfaces; very Small Angle X-ray Scattering and Wide Angle X-ray Diffraction in polymers, Buckminsterfullerenes and other large feature systems; and time resolved element and valence specific single crystal scattering. This is an interagency cooperative funding of the ChemMatCARS Collaborative Access Team at APS in partnership with the National Science Foundation.

UNIVERSITY OF NEBRASKA
Lincoln, NE 68588-0113

383. FUNDAMENTAL STUDIES OF NOVEL PERMANENT MAGNET MATERIALS
D. J. Sellmyer, Department of Physics
(402) 472-2407 02-2 $75,000

Research to advance the understanding of the magnetic rare earth - transition metal compounds and alloys that have high Curie temperatures and large magnetization. The materials studied usually are based on iron and light rare earths, and are generally ternary or higher order alloys with unusually complex, anisotropic structures. Investigated are Fe-rich phases which have been nitrogenated or carbonated to enhance their magnetic properties, new phases reached by intermediate metastable phases via melt spinning, materials produced by mechanical alloying in a high energy ball mill under inert atmosphere, and nanostructured and nanocomposite films made by sputtering techniques. Extensive characterization of the materials by comprehensive experiments which include X-ray and neutron diffraction, electron microscopy, dc and ac magnetic susceptibility, Fe^{57} Mossbauer, and photoemission. Spin-polarized, self-consistent electronic structure calculations performed to compare with the experimental results. Research performed in close collaboration with work at the University of Delaware.

NEW JERSEY INSTITUTE OF TECHNOLOGY
Newark, NJ 07102-1982

384. INVESTIGATION OF THE TRANSPORT MECHANISMS IN CMR MATERIALS: LOCAL STRUCTURAL EFFECTS
T.A. Tyson, Department of Physics
(201) 642-4681 01-3 $100,000

Fundamental aspects of transport mechanisms in magnetoresistive materials. Metal-insulator transition in $La_{1-x}A_xMnO_3$ as a function of doping (x) and divalent cation (A). Changes in local structure due to applied magnetic fields and pressure. Direct measurement of total magnetoactive spin. Optimization of local structure for device use. Basic understanding of electron transport in transition metal oxides.

UNIVERSITY OF NEW MEXICO
Albuquerque, NM 87131

385. PARTICLE-INDUCED AMORPHIZATION OF COMPLEX CERAMICS

R.C. Ewing, Department of Geology
(505) 277-4163 01-1 $0 (0 months)

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

NORTH CAROLINA A&T STATE UNIVERSITY
551 McNair Hall
Greensboro, NC 27411

386. MICROSTRUCTURE - PROPERTY CORRELATIONSHIPS IN OXIDE HETEROSTRUCTURE

C.B. Lee, Department of Electrical Engineering
(910) 334-7760 01-1 $171,989

Processing and characterization studies to understand microstructure-property correlationships in ferroelectrics and superconductor heterostructures. Use of pulsed laser ablation technique to fabricate these heterostructures. Optimization of laser and processing parameters. Atomic level characterization with STEM-Z HRTEM, Auger, etc. Electrical property characterization for sharp resistive transitions and low noise characteristics in high T_c materials.

NORTH CAROLINA CENTRAL UNIVERSITY
Durham, NC 27707

387. STUDIES OF THE STRUCTURE AND PROPERTIES OF ORGANIC MONOLAYERS, MULTILAYERS AND SUPERLATTICES

J. M. Dutta, Department of Physics
(919) 683-6452 02-2 $0 (0 months)

Study the mechanical properties of organic monolayers on the surface of water (Langmuir films). Determine the microscopic structure of such films and of multilayers formed on repeatedly dipped substrates (Langmuir-Blodgett films) using ellipsometry, conventional and synchrotron X-rays. Mechanical property studies directed toward shear response, and important but previously neglected structural property. Diffraction technique, involving external reflection at the monolayer surface, will be used to determine film structure. Finally, the loss of certain symmetry elements of surface phases studied by observing the rotation of plane polarized light incident normal to the surface. A search for this effect within the so-called liquid expanded-liquid condensed region, may indicate a liquid crystal phase.

NORTH CAROLINA STATE UNIVERSITY
Raleigh, NC 27695-8202

388. RESEARCH AT, AND OPERATION OF THE MATERIALS SCIENCE X-RAY BEAMLINE (X-11) AT THE NSLS

D. E. Sayers, Department of Physics
(919) 515-4453 02-2 $340,000

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

389. ELECTRONIC BAND STRUCTURES AND CRYSTAL PACKING FORCES FOR LOW-DIMENSIONAL SOLID STATE MATERIALS

M. H. Whangbo, Department of Chemistry
(919) 515-3464 03-1 $110,000

Theoretical investigation of the electronic and structural properties of various low-dimensional solid state materials, which include: (1) organic conducting and fullerene salts, (2) cuprate superconductors, and (3) transition-metal compounds. The primary techniques for the investigation are tight-binding electronic structure calculations and ab initio self-consistent-field/molecular-orbital (SCF-MO) approaches. The main objectives of the project are to search for structure-property correlations which serve to govern the physical properties of the various materials, and to develop a library of efficient computer programs for the calculation of the physical properties of low-dimensional solid state materials. The work also involves the rational interpretation of STM and AFM images of various layered materials on the basis of density plot calculations. The research also includes the study of images obtained by STM and AFM of solid surfaces and self-assembled overlayers.

390. THEORETICAL STUDIES OF SURFACE REACTIONS ON METALS AND ELECTRONIC MATERIALS

J. L. Whitten, Department of Chemistry
(919) 515-7277 03-1 $90,000

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

UNIVERSITY OF NORTH CAROLINA
CB#3255 Phillips Hall
Chapel Hill, NC 27599-3255

391. THEORIES OF DISORDER AND CORRELATIONS IN FULLERIDES

J. Lu, Department of Physics and Astronomy
(919) 962-3012 02-3 $46,603

Theoretical models for the effects of disorder and correlation on the electronic and superconducting properties of alkali doped fullerides AxC_{60} large fullerides and nanotubes will be formulated and studied. Correlations are to be incorporated utilizing degenerate Hubbard model extentions of previously constructed tight binding representations for the electronic structure. Disorder, both of the C_{60} molecules and of alkali positions, will be studied using Kubo-Greenwood transport theory. The superconducting state will be examined utilizing the real space deGennes-Bogoliubov equations.

392. SOLID-STATE VOLTAMMETRY AND SENSORS IN GASES AND OTHER NON-IONIC MEDIA

R. W. Murray, Department of Chemistry
(919) 962-6295 03-2 $81,500

This project is based on using microelectrode voltammetry for design and application of quantitative electrochemical tranpsort and kinetics experiments to semi-solid and solid redox phases. The experiments include transport and electron transfer reactions of electron donor/acceptor solutes and surfaces in polymeric solvents and liquid crystalline phases. The goals of this project include: (i) developing the necessary miniaturized electrode methdologies, cells, and requisite theory for quantitative voltammetry in rigid media, (ii) exploring important characteristics of homogeneous and heterogneous electron transfer reaction dynamics in rigid environments, in particular how the dynamics of "outer sphere" redox couples respond to rigidification of their surroundings, (iii) exploring polymer-phase transport, including polymer-in-polymer diffusion of redox-labelled poly-ethers, anisotropic transport in liquid crystalline phases and polymers, and coupling between slow diffusion and homogeneous electron transfers, and (iv) learning to dynamically mainupulate diffusion rates of redox sites within polymer electrolytes so as to fashion ultrathin, electrically conducting mixed valent layers by freezing the concentration gradients that are electrolytically generated at electrodes. We have recently succeeded in fashioning an example of a frozen gradient system, from a poly-ether-derivatized viologen.

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

393. IMPURITY-INDUCED CORROSION AT GRAIN BOUNDARIES, METAL-OXIDE INTERFACES AND OXIDE SCALES

J.A. Kelber, Department of Chemistry
(817) 565-3265 01-3 $103,704

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

NORTHEASTERN UNIVERSITY
110 Forsyth Street
Boston, MA 02115

394. COMPUTER MODELING OF SOLIDIFICATION MICROSTRUCTURE

A.S. Karma, Department of Physics
(617) 373-2929 01-5 $70,561

Anomalous eutectics, dendrite fragmentation and eutectic colony formation in ternary alloys are theoretically studied. The phase field method will be used for the computation of the solidification morphology. An adaptation of the classic Rayleigh instability will be applied towards dendrite fragmentation. This may have a significant application towards predicting the microstructure of castings. Research on anomalous eutectic structure will help understand the microstructure of eutectic solders.

395. MICROSCOPIC MECHANISMS FOR FRICTION

J. Sokoloff, Physics Department
(617) 373-2931 02-3 $30,000 (3 months)

Fundamental mechanisms of dissipation are to be studied for two surfaces sliding in contact: i.e. the basic mechanisms of sliding friction. A dual approach will use both analytic and computer studies performed on dialyzed models specifically designed to elucidate operative effects coupled with molecular dynamics simulations of more realistic models perfomed to uncover physical principles involved. Three main areas will be examined: (1) a comparison of phonon generation and electronic excitations as loss mechanism; (2) the effect of surface defects; and (3) modifications to be anticipated when the solids become sufficiently small as to exhibit finite size effects.

NORTHWESTERN UNIVERSITY
2225N. Campus Drive
Evanston, IL 60208

396. GRAIN BOUNDARY PHENOMENA IN SOLUTE DOPED SRTI0$_3$ BICRYSTALS

V.P. Dravid, Department of Materials Science and Engineering
(847) 467-1363 01-1 $105,630

Atomic structure of acceptor/donor doped grain boundaries in $SrTi0_3$, including the presence, extent, occupancy and associated effects of solute enrichment. Direct determination of the presence, sign, magnitude and spatial extent of grain boundary charge and associated space-charge in doped grain boundaries. Deviation of double Schottky barrier parameters for doped grain boundaries. Investigation of interface dynamics under applied current or field across grain boundaries using in-situ TEM I-V probe and in-situ FEG SEM experiments.

397. POINT DEFECTS AND TRANSPORT AT INTERFACES IN OXIDES

T. O. Mason, Department of Materials Science and Engineering
(847) 491-3198

D. E. Ellis, Department of Physics and Astronomy
(847) 491-3553

J. B. Cohen, Department of Materials Science and Engineering
(847) 491-5220 01-1 $199,519

Investigations of defect structures and electronic transport properties at/near interfaces -- external (surfaces) and internal (grain boundaries) -- in the transition metal oxides, Fe_20_4, Zn0, and in the lanthanide, $Ce0_2$. This is an interdisciplinary study involving X-ray diffraction (glancing incidence diffraction and diffuse scattering), neutron scattering, equilibrium and transient electrical property measurements, and first principals electronic structure theory.

398. ATOMIC STRUCTURE AND CHEMISTRY OF INTERNAL INTERFACES

D. N. Seidman, Department of Materials Science and Engineering
(847) 491-4391 01-1 $0 (0 months)

Fundamental relationships between structures and chemical compositions of metal/ceramic heterophase interfaces. Transmission electron microscopy, high resolution electron microscopy, analytical electron microscopy and atom-probe field-ion microscopy are utilized to study the structure and chemistry of metal/ceramic interfaces. The use of ternary alloys allows for the possibility of studying solute-atom segregation effects at heterophase interfaces; this is an area where very little information exists. Trapping of hydrogen at heterophase interfaces is studied via atom probe microscopy. Some of the systems being studied are: Cu/Mg0, Ni/Cr_20_3, Cu/Be0, Cu/Ni0, Cu/Mg, $Ta(W)/Hf0_2$, $Fe(Sn)/Al_20_3$, $Fe(P)/Al_20_3$, $Fe(Ni)/Al_20_3$, $Ni0/NiCr_20_4$ $Ni(Al)/NiAl_20_4$, Pd(H)/Mg0 and Cu(H)/Mg0. The atom probe measurements, in conjunction with different electron microscopies, yield unique atomic scale information about these heterophase interfaces.

399. ATOMIC SCALE CHEMISTRY AND STRUCTURE OF CERAMIC/METAL INTERFACES

D.N. Seidman, Department of Materials Science and Engineering
(847) 491-4391 01-1 $129,948

The characterization of solute-atom segregation at ceramic/metal interfaces is addressed through atom-probe field ion and tomographic atom probe microscopies, high-resolution electron and scanning transmission electron microscopies, and spatially resolved electron-energy-loss spectroscopy. Theoretical studies involving both ab initio electronic structure calculations and Monte Carlo and molecular dynamics simulations are used to complement the experimental studies.

400. A STUDY OF DEFORMATION MECHANISMS IN NANOCRYSTALLINE METALS BASED ON THEIR MECHANICAL BEHAVIOR UNDER VARIOUS STATES OF STRESS

J. R. Weertman, Department of Materials Science and Engineering
(847) 491-5353 01-2 $86,249

The compressive, microhardness, fatigue and creep properties of nanocrystalline metals and alloys will be studied using improved processing that decreases the flaw population. The structure of the materials will be characterized using X-ray diffraction, small angle neutron scattering and TEM.

401. PLASMA, PHOTON, AND BEAM SYNTHESIS OF DIAMOND FILMS AND MULTILAYERED STRUCTURES

R. P. H. Chang, Department of Materials Science and Engineering
(847) 491-3598 01-3 $73,587

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

402. STRUCTURE AND PROPERTIES OF EPITAXIAL OXIDES

B. W. Wessels, Department of Materials Sciences and Engineering
(847) 491-3219 01-3 $74,705

Electronic, optical and nonlinear optical properties of rare-earth doped thin film perovskite oxides, $SrTiO_3$, $BaTiO_3$, their solid solutions, and rare-earth doped niobates; metalorganic chemical vapor deposition. Effect of rare-earth impurities on electrical and optical properties; Hall effect measurements, thermopower measurements, photoluminescence spectroscopy, photoluminescence decay, and transient photocapacitance spectroscopy. Structure and composition; high resolution transmission electron microscopy, analytical electron microscopy, and X-ray diffraction.

403. DEVELOPING IMPROVED RELATIONSHIPS BETWEEN MICROSTRUCTURE AND CREEP AND SHRINKAGE OF CEMENT-BASED MATERIALS

H. Jennings, Department of Civil Engineering
(847) 491-4858 01-5 $92,780

Study of some of the causes of cracking, particularly of creep and drying shrinkage in cement-based materials. Determination of microscopic stress and strain distributions under various loads and drying conditions for a variety of cement admixtures using an Environmental Scanning Electron Microscope combined with an Image Intensity Mapping Technique developed for this purpose.

404. DEVELOPMENT OF INSTRUMENTATION FOR SURFACE, INTERFACE, AND THIN FILM SCIENCE AT THE ADVANCED PHOTON SOURCE

M. J. Bedzyk, Department of Materials Science and Engineering
(708) 491-3570 02-2 $100,000 (11 months)

Construction and implementation of the DuPont-Northwestern-Dow Collaborative Access Team (DND-CAT) Beamlines at the Advanced Photon Source will be performed. Research is aimed at the structure and composition of surfaces, interfaces and thin films.

405. DEVELOPMENT OF X-RAY FACILITIES FOR MATERIALS RESEARCH AT THE ADVANCED PHOTON SOURCE

M. J. Bedzyk, Department of Materials Science and Engineering
(847) 491-3570 02-2 $186,096

Development of analytical instrumentation for standing wave X-ray experiments to be used on the Du-Pont-Northwestern-Dow Collaborative Access Team (DND-CAT) Beamline end stations at the Advanced Photon Source for research on the structure of advanced materials.

406. ENERGETICS, BONDING MECHANISM AND ELECTRONIC STRUCTURE OF CERAMIC/CERAMIC AND METAL/CERMAIC INTERFACES

A. J. Freeman, Department of Physics and Astronomy
(847) 491-3343 02-3 $70,000

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.

407. X-RAY SCATTERING STUDIES OF LIPID MONOLAYERS

P. Dutta, Department of Physics & Astronomy
(847) 491-5465 03-3 $105,000

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 structure after shear response. Diffraction techniques, involving external reflection at the monolayer surface, used to determine film structure.

UNIVERSITY OF NOTRE DAME
Notre Dame, IN 46556

408. SELF-ORGANIZED SUPERLATTICE FORMATION IN TETRAHEDRALLY-BONDED SEMICONDUCTOR ALLOYS

J.K. Furdyna, Department of Physics
(219) 631-6741 01-3 $117,864

Experimentally study and modeling effort of growth phenomena responsible for the formation of periodic vertical phase separation (self-organized superlattices) in III-IV and II-IV semiconductor alloys. $GaAs_{1-x}Sb_x$, $Ga_{1-y}Al_yAs_{1-x}Sb_x$, $CdSe_{1-x}Te_x$, $Zn_{1-y}Cd_ySe_{1-x}Te_x$, and other systems to be studied. Samples grown on vicinal cut substrates (e.g., GaAs) and characterized by TEM/TED to obtain structural details. High accuracy XRD studies to determine spatial extent of modulation. Optical studies to determine the nature and perfection of quantum well effects. Continuum and Monte Carlo modeling of growth and phase separation processes.

409. EXPERIMENTAL FACILITIES FOR IN-SITU STUDIES OF MATERIALS AND PROCESSES AT THE ADVANCED PHOTON SOURCE

B. A. Bunker, Department of Physics
(219) 631-7432 02-2 $0 (0 months)

Construction and implementation of the Materials Research Collaborative Access Team (MR-CAT) Beamlines at the Advanced Photon Source will be performed. Research is aimed at materials and processes under extreme conditions of temperature, field, processing or geometrical confinement.

410. SINGLE ELECTRON TUNNELING
S. T. Ruggiero, Department of Physics
(219) 631-7463 02-2 $0 (0 months)

This experimental program examines the so-called "Coulomb Staircase" effect arising from single electron tunneling into small metallic clusters. The clusters, consisting of only a few atoms, can thus be examined for bond lengths and basic electronic structure properties. The project focuses on opportunities to observe quantum effects in the important mesoscopic and few-atom regime.

OHIO STATE UNIVERSITY
2041 College Road
Columbus, OH 43210-1178

411. EXPERIMENTAL AND THEORETICAL STUDY OF DISLOCATION PROCESSES AND DEFORMATION BEHAVIOR IN B2 INTERMETALLIC COMPOUNDS OF THE (FE,NI) AL PSEUDOBINARY SYSTEM
M.J. Mills, Department of Materials Sciences and Engineering
(614) 292-2553 01-2 $114,962

Mechanical properties and characterization of the dislocation microstructure of single crystals of several compositions within the (Fe,Ni)-Al pseudobinary system. Systematic examination of alloys bridging the behavior from FeAl to NiAl. Mechanical testing of the single crystals including constant strain-rate, strain-rate change and predeformation/temperature change experiments. Detailed characterization of the dislocation structures using both weak beam and high resolution transmission electron microscopy. Fundamental understanding of the complex dislocation processes which control the deformation behavior in these B2 compounds.

412. INTERFACE DIFFUSION AND DEEP LEVEL FORMATION OF SIC AND OTHER WIDE GAP MATERIALS
L.J. Brillson, Department of Electrical Engineering
(614) 292-8015 01-3 $118,000

Fundamental aspects of interface phenomena in wide bandgap materials. Interface diffusion in metal/semiconductor junctions. Schottky barrier formation, heterojunction band offsets, and optical and electronic features of small scale impurity confinement. Experimental measurements using XPS, AES, SIMS, CLS, PLS, and other surface sensitive techniques. Surface chemical composition before and during interface formation and as a function of annealing temperature and period.

413. THEORIES OF HEAVY FERMION NORMAL STATE
D. Cox, Department of Physics
(614) 292-0620 02-3 $55,288 from prior year

The normal state properties of heavy fermion materials are studied. Emphasis is in three areas: (i) Monte Carlo studies of the two-channel Kondo lattice in infinite dimensions. Interest is the possible non-Fermi liquid behavior and precision of simpler appoximations. (ii) Model uranium impurities in the extreme mixed valence phas where f_2 and f_3 configurations are nearly equally occupied. Interest is the crossover between ground state nature and implications for the non-linear susceptibility. (iii) Melting of local density approximation calculations of hybridization matrix elements and host electronic structure with dynamic many body treaments of the f-electron sites.

414. STRONGLY INTERACTING FERMION SYSTEMS
J. W. Wilkins, Department of Physics
(614) 292-5193 02-3 $108,000

The study of the optical properties of insulators with enhancements (i) parallel computation of the quasi-particle band structures with attentionto defects and superlattices; (ii) optical properties in strong magneticfields. Work on strongly correlated 'atoms', in addition to the program on transition metals, will involve the study of the (iii) use of pseudopotentials in atoms/molecules, (iv) use of non-orthogonal orbits to enhance the effectiveness or state selection, (v) real-time dynamics of atoms and quantum dots in the presence of ultrafast, intense laser pulses. In addition, work on many-body effects in bulk or limited dimensional systems will with (vi) realistic treatment of electron-electron scatteringin magnetic transiton metals and (vii) combined effect of electron-phonon and impurity scattering on transport effects.

415. SYNTHESIS OF MOLECULAR/POLYMER BASED MAGNETIC MATERIALS

A. J. Epstein, Department of Physics
(614) 292-1133/3704 03-1 $175,000 (10 months)

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

OHIO UNIVERSITY
Athens, OH 45701-2979

416. ELECTRONIC INTERACTIONS IN CONDENSED MATTER SYSTEMS

S. E. Ulloa, Department of Physics and Astronomy
(614) 593-1729 02-3 $55,000

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.

OLD DOMINION UNIVERSITY
Norfolk, VA 23529

417. DYNAMICS OF SURFACE MELTING

H. Elsayed-Ali, Department of Electrical and Computer Engineering
(804) 683-3741 03-3 $125,000 (11 months)

Experimental investigation of the dynamics of surface melting for metallic single crystals and thin epitaxial metal films. Time-resolved reflection high energy electron diffraction (RHEED), with picosecond time resolution, is used to study the surface melting upon fast heating and cooling. Observation of the time evolution of lattice expansion during ultrafast heating. Detailed studies of superheating (retention of near-surface structure above the bulk melting temperature) and the dynamics of melting. Examples of systems investigated are surfaces of Pb and Bi, expitaxial films of Pb on Si, and low vapor pressure alloys for comparison with static studies.

ORDELA INC.
1009 Alvin Weinberg Drive
Oak Ridge, TN 37830

418. DEVELOPMENT AND INSTALLATION OF A HIGH RESOLUTION POSITION SENSITIVE 40 CM X 40 CM GAS DETECTOR FOR SANS APPLICATIONS AT IPNS

M. K. Kopp,
(423) 483-8675 02-2 $200,000

The new small angle neutron diffractometer (SAND) instrument at the Intense Pulsed Neutron Source, Argonne National Laboratory will be upgraded through the development and installation of a state-of-the-art position sensitive area detector with higher spatial resolution, greater stability, and with capability for higher count rates.

OREGON STATE UNIVERSITY
Corvallis, OR 97331

419. HYPERFINE EXPERIMENTAL INVESTIGATIONS OF POINT DEFECTS AND MICROSCOPIC STRUCTURE IN GROUP IV OXIDE CERAMICS

J.A. Gardner, Department of Physics
(541) 737-3278   01-1 $16,644

Support is provided for an assistant to Professor Gardner and to indirectly support Perturbed Angular Correlation Spectroscopy work on tetragonal zirconia and ceria. Research objectives include further examination of tetragonal zirconia to measure the dependence of the density of free double positive oxygen vacancies on the partial pressure of oxygen and on grain size between temperatures of 1000 and 1400C and high temperature NMR measurements to see if the tetragonal $Zr0_2$ has a domain superstructure as possibly indicated by previous PAC spectroscopy measurements.

420. COORDINATOR ACTIVITIES FOR DOE-CSP METAL FORMING PROJECT

M.E. Kassner, Department of Mechanical Engineering
(541) 737-7023   01-5 $24,500

The Metals Forming Project of the Center for Excellence for the Synthesis and Processing of Advanced Materials has as its first objective scientific understanding of phenomena relating to the forming of aluminum alloys for commercial (especially automotive) applications. The second objective is developing equations that predict the mechanical behavior of aluminum alloys during and after a complicated series of thermal and mechanical processing steps. Emphasis is currently on recrystallization. The support provided here is to fund the coordinator's efforts in leading and integrating the distributed research team at eight DOE laboratories together with university and industrial collaborators to serve the needs of basic and applied research in the area of aluminum and eventually other metal forming processes.

421. UPGRADE OF THE HIGH-RESOLUTION NEUTRON POWDER DIFFRACTOMETER AT THE HFBR AT BNL

A. W. Sleight, Department of Chemistry
(541) 737-6749   02-1 $9,039 (0 months)

Upgrade of the High Resolution Neutron Powder Diffractometer at the High Flux Beam Reactor to increase the number of available wavelengths and provide an even higher resolution than is presently available.

UNIVERSITY OF OREGON
Eugene, OR 97403-1274

422. NANOSCALE MATERIAL PROPERTIES: SOFT X-RAY SPECTROSCOPY AND SCATTERING

S. D. Kevan, Department of Physics
(541) 346-4742   02-2 $126,000

This research program probes the structure of materials, surfaces, and interfaces on a variety of length and energy scales using soft X-rays. New focus is on understanding the interactions between adsorbates on a surface; diffusion and nucleation in materials prepared as synthetic multilayers and then reacted; fluctuation phenomena of surface diffusion, distruction of long range order, and polymers. Focus on Fermi surface problems and quasi-2D transition metal phosphochalcogenide materials will continue at a diminished rate of progress.

423. NONLINEAR OPTICAL STUDIES OF SEMICONDUCTOR/LIQUID AND LIQUID INTERFACES

G. L. Richmond, Department of Chemistry
(541) 346-4635   03-2 $90,000

Studies of interfacial structure and dynamics using second harmonic generation (SHG) and hyper-Raman scattering. Development of SHG for monitoring electrochemical reactions on a nanosecond to femtosecond timescale, correlation of surface structure with electron transfer kinetics, thin-film nucleation and growth, and analyses of the structure and reactive role of surface defects.

PENNSYLVANIA STATE UNIVERSITY
104 Davey Laboratory
University Park, PA 16802

424. VIBRATIONAL AND ELECTRONIC PROPERTIES OF FULLERENE AND CARBON-BASED THIN FILMS

J. S. Lannin, Department of Physics
(814) 865-9231   01-1 $102,200

Study of nanoscale systems of carbon-based solids using conventional multichannel and interference Raman scattering (IERS) and vibrational and electronic high resolution electron energy loss spectroscopy (HREELS). The three forms of carbon are: 1) fullerene-based, metal-C_{60} systems; 2) very small, 1-2nm, isolated nanocrystalline graphite-derived particles on surfaces; and 3) amorphous diamond-like carbon (DLC). Pulsed laser and vacuum arc plasma deposition techniques together with multilayer methods to make A_xC_{60} materials (where A = Na, K, and Rb). Thin and ultrathin film studies to clarify the effects of alkali type and concentration on structural disorder and electron-phonon coupling.

425. CONTROLLED SYNTHESIS OF METASTABLE OXIDES UTILIZING EPITAXIAL STABILIZATION

D. Schlom, Department of Materials Science and Engineering
(814) 863-8579 01-1 $125,162

Controlled growth of multi-component oxides using MBE to achieve epitaxial stabilization of metastable phases. Synthesis and characterization of three oxides: a ferroelectric Aurivillius phase with the general formula Bi_20_2 $(A_{n-1}B_n0_{3n+1})$; and two superconducting oxides, a $CuBa_2(y,Ca)_{n-1}Cu_n0_{2n+3}$, and a metastable Ruddlesden-Popper phase with the general formula $(Ba,K)_{n+1}(Pb,Bi)_n0_{3n+1}$. A broad array of *in situ* and *ex situ* characterization techniques will be used to realize the film growth and measure their physical properties.

426. BASIC UNDERSTANDING OF WELDMENT COMPOSITION AND MICROSTRUCTURE FROM FUNDAMENTALS OF TRANSPORT PHENOMENA

T. DebRoy, Department of Materials Science and Engineering
(814) 865-1974 01-5 $214,791

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

UNIVERSITY OF PENNSYLVANIA
3231 Walnut Street
Philadelphia, PA 19104

427. SCANNING TUNNELING MICROSCOPY AND SPECTROSCOPY OF CERAMIC INTERFACES

D. A. Bonnell, Department of Materials Science and Engineering
(215) 898-6231 01-1 $74,209

Investigation of the effects of interfacial structure and chemistry on the local electrical properties at grain boundaries in ceramics using scanning tunneling microscopy (STM) and transmission electron microscopy (TEM). Develop improved understanding regarding the imaging of large band gap structures in STM. Measurements and calculations of space charge at interfaces. $SrTi0_3$ is used as the model oxide.

428. STRUCTURE AND DYNAMICS IN LOW-DIMENSIONAL GUEST-HOST SOLIDS

J.E. Fischer, Department of Materials Science and Engineering
(215) 898-6924 01-1 $149,588

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

429. ATOMISTIC STUDIES OF INTERFACES IN MULTI-COMPONENT SYSTEMS

V. Vitek, Department of Materials Science and Engineering
(215) 898-7883 01-1 $78,602 (6 months)

Atomistic computer simulation studies of grain boundaries in binary ordered and disordered alloys. Investigation of grain boundaries with segregated solutes. Study of grain boundary and metal-ceramic interface electronic structure. Methods of calculation of interatomic forces.

430. OXIDE CERAMIC ALLOYS AND MICROLAMINATES

I-W. Chen, Department of Materials Science and Engineering
(215) 898-8337 01-2 $105,591

Solute-defect interactions and segregation; CeO_2, Y_2O_3 and ZrO_2 host oxides; solid solutions with oxides of divalent Mg, Ca and Sr, trivalent Sc, Yb, Y, Gd and La, tetravalent Ti and Zr, and pentavalent Nb and Ta. Static grain growth, dynamic grain growth and related mechanical phenomena; mechanisms for solute drag, solute-defect interactions; static grain growth experiments, grain boundary mobility, compression tests, dislocation creep; construction of stress-strain constitutive relation incorporating grain growth; microstructural and microchemical characterization. Densification kinetics, microstructure development, grain boundary mobility; doped solid solutions; effect of solute drag on sintering of second phase ceramics; effect of initial porosity. Deformation and fracture of ceramic slips. Plasticity induced interface instabilities. Sintering and microstructure development of bimaterials and compositionally grated materials. Strength and fracture of compositionally graded materials. Strength and fracture of layered, graded, and multiply connected cellular composites.

431. TWINNING IN LAVES PHASES BY SYNCHROSHEAR: ATOMIC MECHANISMS AND COMPOSITIONAL CONTROL

D.P. Pope, Department of Materials Science and Engineering
(215) 898-9837

D. E. Luzzi, Department of Materials Science and Engineering
(215) 898-8366 01-2 $107,000

The atomic mechanisms of twinning in the Laves phases will be investigated through examination of Nb doped HfV and similar compounds. A combination of mechanical testing, high resolution electron microscopy, single crystal growth and compositional control will be used to help evaluate whether a thermal barrier to twinning exists and whether the extent and nature of twinning can be altered through changes in loading state and changes in compositions.

432. COMPLETION OF AN UNDULATOR-BASED X-RAY SCATTERING FACILITY FOR MATERIALS RESEARCH ON COMPLEX FUNDS

J. K. Blasie,
(215) 898-6208 02-2 $1,573,950

Completion of construction by the Complex Materials Collaborative Access Team (CMC-CAT) at the Advanced Photon Source of a second undulator-based beamline with focusing optics, allowing for parallel operation of two focusing beamlines on the undulator-magnet source, and an additional endstation with instrumentation optimized for grazing incidence X-ray scattering from liquid surface/interfaces and for small angle X-ray scattering. Research will be aimed at structural characterization of complex materials, including complex fluids, self-assembling systems, surfaces and interfaces, and heterogenious materials.

433. CONDENSED MATTER PHYSICS AT SURFACES AND INTERFACES OF SOLIDS

E. Mele, Department of Physics
(215) 898-3135 02-3 $65,000

Theoretical investigations of electronic transport phenomena in nanoscale molecular conductors will be performed. Investigation of the interplay between shape fluctuations and electronic transport in these structures, with emphasis of the effects of local geometry on the propagation and scattering of a quantum particle within the tangent plane for these systems. The theory will be applied to transport phenomena in materials developed from carbon nanotubes, and to a large class of related molecular conductors. Theoretical investigation of magnetic ordering in the fullerides doped at low density, and in particular on understanding the competing roles of frustration and disorder for controlling the magnetic states in these systems.

UNIVERSITY OF PITTSBURGH
Pittsburgh, PA 15260

434. THE PHYSICS OF PATTERN FORMATION AT LIQUID INTERFACES

J. V. Maher, Department of Physics and Astronomy
(412) 624-9007 02-2 $115,000

The formation of patterns at liquid interfaces and the behavior of interfaces inside disordered systems is investigated in: 1) a study of the changes in patterns available to the growth of a macroscopic interface when that interface is grown over one of a variety of "microscopic"lattices, 2) a study of dissolved particles in mixed solvent, with attention paid to interactions and 3) an investigation of the sedimentation of particles in a quasi-two-dimensional viscous fluid, and of the relationship between the dynamics of the flow and of the roughness of the resulting surface of settled particles.

435. PATTERN FORMATION IN POLYMER FILMS

A. C. Balazs, Department of Materials Science and Engineering
(412) 648-9250 03-2 $130,000

Computer simulations and theoretical models to examine how architecture and morphology affect the properties of polymers at surfaces and interfaces. 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 may yield the optimal interfacial structure for such applications as patterning, adhesion and film growth. The approach involves the use of statistical mechanics, molecular dynamics and Monte Carlo computer simulations to model the polymer-surface interactions. These studies can allow the determination of how varying molecular structure or the chemical environment affects the properties of the interface.

POLYTECHNIC UNIVERSITY
Six MetroTech Center
Brooklyn, NY 11201

436. DEFORMATION, ANOMALOUS HARDENING AND DISLOCATION STRUCTURE IN SINGLE CRYSTAL GAMMA-TIAL

S.H. Whang, Department of Metallurgy and Materials Science
(718) 260-3144 01-2 $96,503

Deformation and microstructural characterization of single crystal TiAl to elucidate mechanical property-microstructure relationships, in particular with regard to anomalous hardening. Elastic constants and TEM observations, of dislocation structures will be employed to develop theoretical models to explain the deformation mechanisms.

437. SCANNING TUNNELING MICROSPECTROSCOPY OF SOLIDS AND SURFACES

E. L. Wolf, Department of Applied Mathematics and Physics
(718) 260-3850 02-2 $96,000

This combined theoretical and experimental program utilizes Scanning Tunneling Spectroscopy as the preferred experimental technique to examine electronic properties and processes at the surface and to relate them to structure. Primary interests are the superconducting pairing mechanism; proximity effects in cuprate superconductors and overlayed metal films; fluctuations in the order parameter, and the correlation of fluctuations with magnetic excitations. Theoretical effort deals with the coupled Josephson junction view of the cuprate superconductors and interactions with the magnetic field.

438. STRONGLY CORRELATED ELECTRONICS MATERIALS

P. Riseborough, Department of Physics
(718) 260-3675 02-3 $57,000

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 08540

439. MECHANICAL PROPERTIES OF GELS

G. Scherer, Department of Civil Engineering
(609) 258-5680 01-2 $125,000

Mechanical properties of gels with a wide range of pore structures. Properties and structures will be followed during the coarse of drying and shrinkage. Several complementary techniques will be employed to follow the evolution of microstructure and mechanical behavior. The main physical parameter of interest is the elastic modulus. Measurement techniques include oscillatory rheometry, shear wave propagation, dynamic light scattering, and beam bending. An attempt will be made to compare and relate the results from these methods as it applies to the behavior of sol-gels. The complete characterization of the elastic properties will afford testing of the power law dependence of elastic modulus on the volume of solids in the microstructure. Computer modeling of network structures will be employed in order to elucidate the structural features that give rise to the observed mechanical behavior.

440. THERMOCHEMICAL STUDIES OF THE STABILITY OF NITRIDES AND OXYNITRIDES

A. Navrotsky, Department of Geological and Geophysical Sciences
(609) 258-4674 01-3 $0 (0 months)

The basic thermodynamic properties of nitrides and oxynitrides and the relations among energetics, structure, and bonding are far less well known than for oxides. The goals of this work are to develop high temperature reaction calorimetric techniques for measuring enthalpies of formation of nitrides and oxynitrides, to determine energetics of sialons and ternary nitrides, and to formulate thermochemical systematics useful for predicting phase stability, materials compatibility, and the synthesis of new compounds.

441. DEVELOPMENT OF ADVANCED X-RAY SCATTERING FACILITIES FOR COMPLEX MATERIALS

P. Eisenberger, Princeton Materials Institute
(609) 258-4580 02-2 $0 (0 months)

Construction and implementation of the Complex Materials Collaborative Access Team (CMC-CAT) Beamline at the Advanced Photon Source will be performed. Research is aimed at structural characterization of complex materials. Included materials include complex fluids, self-assembling systems, surfaces and interfaces, and heterogeneous materials.

442. STRUCTURE AND STEREOCHEMISTRY OF SELF-ASSEMBLED MONOLAYERS

G. Scoles, Department of Chemistry
(609) 258-5570 03-2 $150,000

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

UNIVERSITY OF PUERTO RICO
Facundo Bueso Bldg.
Rio Piedras, PR 00931

443. PARTICLES, PROCESSES AND MATERIALS FOR MODERN ENERGY NEEDS: DEVELOPMENT OF A DOE EPSCOR PROJECT IN PUERTO RICO

B. R. Weiner, Resource Center for Science and Engineering
(809) 765-5170 05-1 $750,000

High energy particle physics, novel thin films materials, and catalytic processes for energy sources and environmental detoxification will continue to be the three thrust areas of the Puerto Rico DOE/EPSCoR Program. The "High Energy Particle Physics" research effort is concentrated on two experiments conducted at Fermi National Laboratory. Both of these experiments, (E687 and E831) study the photo production and decay of particles containing the charm quark. Data collected from the very successful E687 experiment continues to be the subject of intense analyses. The E831 data will be enhanced by significant upgrades to the E687 spetrometer that will allow the analysis of important but weaker events. "Novel Thin Film Materials for Optoelectronics Applications" will be investigating thin films of novel optoelectronics, ferroelectrics, and glass ceramics. Films will be grown using pulsed laser deposition, molecular beam epitaxy, ion beam sputtering, radio frequency sputtering and sol-gel technqiues. Characterization of these films have been achieved by nonlinear optical studies such as laser Raman scattering, luninescence, infrared, static light scattering and photon correlation spectroscopies. "Catalytic Process in Energy Sources and Environmental Detoxification" is organized into two major thrust areas: energy sources and environmental detoxification. The Energy Sources Project will include studies of: (1) high energy intermediates in the gas phase in combustion of fossil fuels, (2) copper metal particles imbedded in a polymer matrix to provide stabilization for highly reactive catalytic sites in modified electrodes,

(3) luminescent metal complexes in layered materials that promote photoinduced charge separation, and (4) silica-based mesoporous materials in an attempt to synthesize other novel materials. The Environmental Detoxification Project will focus on four areas: (1) new solid-liquid phase catalyst, trisopropylsilanol, for detoxification applications of mustard gas analogues and environmmental pollutants, (2) oxidative detoxification of volatile organic compounds in the gas phase, (3) new absorbed photosensitizers; and (4) new catalytic materials for energy-related processes and interests.

PURDUE UNIVERSITY
West Lafayette, IN 47907

444. BEAM LINE OPERATION AND MATERIALS RESEARCH UTILIZING NSLS

G. L. Liedl, Materials Engineering Division
(317) 494-4100 01-1 $254,015

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 beamline at the National Synchrotron Light Source (NSLS). A unique and versatile monochromator provides radiation to a four-circle Huber diffractometer for the basic system. Multiple counting systems are available as well as a low temperature stage, a high temperature stage, and a specialized surface diffraction chamber. The grant covers the operational expenses and system upgrade of this beamline at NSLS for all MATRIX members, and to support part of the research on phase transformation studies, X-ray surface and interface studies.

445. MIDWEST SUPERCONDUCTIVITY CONSORTIUM

A. L. Bement, School of Materials Engineering
(317) 494-5567 01-5 $3,051,000

The Midwest Superconductivity Consortium (MISCON) was formed in response to Congressional direction. The consortium emphasis is in issues of ceramic superconductor synthesis, development, processing, electron transport, and magnetic behavior. Efforts are both theoretical and experimental. The membership includes Purdue University, University of Nebraska, Notre Dame University, Ohio State University, Indiana University, and the University of Missouri-Columbia.

446. X-RAY PHYSICS OF MATERIALS

S. Durbin, Department of Physics
(317) 494-6426

R. Colella, Department of Physics
(317) 494-6426 02-2 $500,000

Development of end stations to be used on the Synchrotron Radiation Instrumentation Collaborative Access Team (SRI-CAT) beamlines at the Advanced Photon Source. Diverse X-ray physics studies including microdiffraction, standing wave applications, imaging optics, resonant nuclear scattering, and magnetic diffraction.

RENSSELAER POLYTECHNIC INSTITUTE
110 Eighth Street
Troy, NY 12180-3590

447. NUCLEATION AND GROWTH OF SEMICONDUCTOR NANOCRYSTALS BY SOLID-PHASE REACTION

T. M. Hayes, Department of Physics; 1W10 SC
(518) 276-8396

P. D. Persans, Department of Physics
(518) 276-8396 02-2 $50,000 (2 months)

Optical and X-ray absorption will be used to study nanocrystals of cadmium chalchogenides during early stages of growth when produced by solid state reaction in borosilicate glasses. For larger nanocrystallites, additional measurements will be made using transmission electron microscopy (provides an excellent calibration), X-ray diffraction, and small angle X-ray scattering. The X-ray probes will establish the calibration of the optical probes that will be used for general scanning purposes. Thereafter, process parameters will be varied to provide examples in appropriate growth ranges for study.

UNIVERSITY OF RHODE ISLAND
317A East Hall
Kingston, RI 02881-0817

448. PHYSICS WITH ULTRACOLD AND THERMAL NEUTRON BEAMS

A. Steyerl, Department of Physics
(401) 792-2204 02-1 $25,000

The methods of surface reflectometry to the use of ultra cold neutrons will be extended. 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. Applications are to magnetic multilayer systems, surfactant effects, polymer films, and to effects influencing neutron lifetimes.

RICE UNIVERSITY
Houston, TX 77251-1892

449. HIGH-RESOLUTION MAGNETIC IMAGING AND INVESTIGATIONS OF THIN-FILM MAGNETISM WITH SPIN-POLARIZED ELECTRON, ION AND ATOM PROBES

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

F. B. Dunning, Department of Physics
(713) 527-8101 02-2 $200,000

Exploitation of unique capabilities in electron spin polarimetry, polarized particle beams, and spin-sensitive electron spectroscopies to develop new imaging spectroscopies that are suitable for high-resolution studies of magnetic domain structures of thin films and multilayers. An existing Scanning Electron Microscope (SEM) will be modified to obtain an SEM with Polarization Analysis (SEMPA), which is estimated to be able to inspect written magnetic domain patterns on a thin film within a 20 to 50 nanometer length scale. Use of an incident beam of spin-polarized low energy He+ ions to develop a Spin-Polarized Ion Neutralization Spectrometer (SPINS) that would be useful to image magnetic domain structures with a spatial resolution of about one micrometer. Application of the SEMPA and SPINS imaging techniques to investigate basic questions of magnetic data storage materials. Studies of ferromagnetic surfaces and thin films by use of Spin-Polarized Metastable (atom) Deexcitation Spectroscopy (SPMDS). Adaptation of existing SPMDS apparatus in order to study the interaction of Rydberg atoms with surfaces.

ROCKWELL INTERNATIONAL CORPORATION
1049 Camino Dos Rios
Thousand Oaks, CA 91362

450. FAILURE MECHANISMS FOR CERAMIC MATRIX TEXTILE COMPOSITES AT HIGH TEMPERATURE

B.N. Cox,
(805) 373-4128 01-2 $130,000

Fundamental aspects of failure in ceramic matrix composites with textile reinforcement at high temperatures. Transition with increasing temperature from multiple cracking to single dominant matrix cracking (localization/delocalization transition) in ceramic matrix composites with creeping fibers. Determining by micromechanical modeling how constituent material properties and fiber architecture control failure mechanisms; including the role of anisotropy in distinguishing failure mechanisms and load redistribution effects in ceramic matrix composites and polymer matrix composites. The micromechanisms of damage in bridging twos in laminates with through-thickness reinforcement.

STATE UNIVERSITY OF NEW JERSEY RUTGERS
Piscataway, NJ 08855

451. THERMODYNAMIC, KINETIC AND STRUCTURAL BEHAVIOR OF SYSTEMS WITH INTERMEDIATE PHASES IN CERAMIC AND METAL SYSTEMS

A.G. Khachaturyan, Department of Mechanics and Materials Science
(908) 932-2888

T. Tsakalakos
(908) 932-4711

S. Semenovskage
(908) 932-4711 01-1 $91,983

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

SOUTH CAROLINA STATE UNIVERSITY
300 College Street, N.E.
Orangeburg, SC 29117

452. PROPERTIES OF DOPED BI-BASED HIGH T_C SUPERCONDUCTORS: PART A

J.E. Payne, Department of Physical Sciences
(803) 536-7111 01-3 $100,000

This involves a systematic substitution of Cu in CuO layers of the 2212 and 2223 phases of high temperature superconductors by transition metals (Fe, Co, Ni, Zn). The issue of whether the superconducting pairing state of the cuprates has d-wave or s-wave orbital symmetry can be addressed by studying the physical properties such as susceptibility, specific heat and transport.

UNIVERSITY OF SOUTH CAROLINA
Columbia, SC 29208

453. DOE/EPSCOR RESEARCH IMPLEMENTATION PLAN RENEWAL

R. E. White, Department of Chemical Engineering
(803) 777-3270 05-1 $550,000

This South Carolina DOE/EPSCoR program will continue the collaborative research efforts of the University of South Carolina and Clemson University in the area of "Electrochemical Power Sources." The thrust of the program is to design and develop new methods for producing improved proton exchange membrane (PEM) fuel cells, pure hydrogen for use in PEM fuel cells, lithium polymer batteries, nickel/metal hydride batteries, and supercapacitors. The research is subdivided into six projects: (1) "Mathematical Modeling of Proton Exchange Membrane Fuel Cells and Stacks" focuses on the primary scientific issues associated with PEM fuel cells and fuel cell stack design, (2) "Hydrogen Storage and Delivery Systems Utilizing Chemical Hydrides" is investigating newly developed chemical hydrides as possible candidates for hydrogen storage and for use with small to medium scale PEM fuel cell applications, (3) "Hydrogen Production via the Direct Cracking of Hydrocarbons" is developing new catalysts and a novel membrane reactor design for the production of hydrogen from hydrocarbon fuels through a process called "direct cracking," (4) "Novel Fluorinated Electrolytes for Batteries and Fuel Cells" is studying novel fluorinated polymer electrolytes with improved properties to enhance the performance of PEM fuel cells and polymer/lithium batteries, (5) "Fiber-Optic Chemical Sensors for In-Situ Battery Diagnostics" is developing in-situ fiber-optic probes designed specifically for use in batteries and fuel cells, and (6) "New Materials Modeling and Design Tools for Capacitors and Batteries" is employing innovative sol-gel and electrochemical synthesis techniques to study carbon-metal oxide composites and carbon-metal electrodes for use as hybrid capacitors. Researchers involved in this last project are also experimenting with electrode development for lithium batteries and molecular level mathematical modeling of electrode materials.

UNIVERSITY OF SOUTHERN CALIFORNIA
Los Angeles, CA 90089

454. FACTORS INFLUENCING THE FLOW AND FRACTURE OF SUPERPLASTIC CERAMICS

T.G. Langdon, Department of Materials Science
(213) 740-0491 01-2 $103,766

Investigation of flow mechanisms and method of optimizing superplastic characteristics in yttria-stabilized zirconia (Y-TZP). Propose to build on earlier work by investigating factors which influence the mechanical properties and overall ductility, including examining the role of impurities or an amorphous grain boundary phase. Three critical experiments: (1) direct measurements of grain boundary sliding using scanning electron microscopy, (2) extend analytical procedure for quantitative measurements of cavity distributions to include cavities of very small sizes (~0.1 micro-2_2), thereby obtaining information on cavity nucleation sites, (3) examine feasibility of using photoacoustic technique as a non-destructive evaluation technique to reveal presence of internal cavitation in Y-TZP samples after superplastic deformation.

SOUTHERN UNIVERSITY
P.O. Box 11746
Baton Rouge, LA 70813

455. USE OF THE CAMD FACILITY FOR THE SCIENCE AND ENGINEERING ALLIANCE

R. Gooden, Department of Chemistry
(504) 771-3994 02-2 $300,000 (11 months)

Initiation and performance of materials sciences research by scientists from member institutions of the Science and Engineering Alliance (SEA) at the J. Bennett Johnston, Sr. Center for Advanced Microstructurals and Devices (CAMD), Louisiana State University, Baton Rouge, Louisiana using existing CAMD beamlines; the long-term goals, following establishment of the materials sciences research program are the design, construction, installation, and use of end stations on existing CAMD beamlines unique to the research programs of the Science and Engineering Alliance (SEA) institutions, and, ultimately the design, construction, and operation of dedicated synchrotron radiation beam lines supporting the research of the SEA member faculties and students. Members of the SEA include Alabama A&M University, Jackson State University, Prairie View A&M University and Southern University and A&M College.

456. MAGNETIC PROPERTIES AND SPECTROSCOPIC STUDIES OF SELECTED RARE EARTH-TRANSITION METAL INTERMETALLIC ALLOYS

R. C. Mohanty, Department of Physics
(504) 771-4130

H. S. Li, Department of Physics
(504) 771-4130 02-2 $85,000

Hard Magnetic alloys of the type $(NdDy)_2(Fe_{14-x-y}Co_xT_z)B_{1-n}C_n$ or $R_2(Fe_{17-x-y-z}Co_xCu_yT_z)C_n$ or $R(Fe,Co,T)_{12}C_n$ will be synthesized and characterized as to their microstructural and magnetic properties. The structural details and crystal field effects will be related to the magnetic properties as a function of various compositions and heat treatments.

STANFORD UNIVERSITY
Stanford, CA 94305-2205

457. STRUCTURAL RELIABILITY OF CERAMICS AT HIGH TEMPERATURE: MECHANISMS OF FRACTURE AND FATIGUE CRACK GROWTH

R. Dauskardt, Materials Sciences and Engineering
(415) 725-0679 01-2 $127,427

Study of the fundamental micromechanisms of cyclic fatigue in several classes of ceramics and ceramic-matrix composites. Subcritical crack growth under cyclic applied loads at temperatures as high as 1400°C. Identification of mechanisms responsible for cyclic fatigue, a study of their temperature dependence, and development of mechanistic models describing fatigue failure. Adaptation and development of life prediction procedures. Ultimate goal of the research is to provide a basis for the design of composite ceramic microstructures with optimum resistance to cyclic fatigue.

458. MECHANICAL PROPERTIES OF THIN FILMS AND LAYERED MICROSTRUCTURES

W. D. Nix, Department of Materials Science and Engineering
(415) 725-2605 01-2 $139,691

Study of the strength and adhesion properties of thin films and metal multilayers. FCC/BCC metal multilayer combinations with a wide range of wavelengths made by sputter deposition. X-ray diffraction studies and substrate curvature measurements of multilayer stresses and TEM for the study of microstructure, defects and interfacial epitaxy. Nanoindentation substrate curvature measurements and bulge testing using a laser interferometer system. Modeling of the strength properties of metal multilayers.

459. STUDIES OF SMALL MAGNETIC STRUCTURES USING NEAR-FIELD MAGNETO-OPTICS

A. Kapitulnik, Department of Applied Physics
(415) 723-3847 02-2 $100,000

The novel technique of Sagnac magnetometry will be used in both the far field and near field modes to study the magnetic microstructure of thin magnetic films and multilayers on a sub-micrometer length scale. With this method, sufficient resolution and sensitivity will be achieved to study the structure of small domains and domain walls. This method has an advantage over other probes such as electron microscopy and atomic force microscopy in that it can be performed in any size magnetic field. This method has had great success in the search for any one superconductivity in the high temperature superconductors. The method does not have the resolution of SEMPA (scanning electron microscopy with polarization analysis), but it is laser based spectroscopy and thus has a much wider range of applicability. The work proposed here will apply a new tool to the study of magnetism and will open a whole new field.

460. ULTRA-LOW TEMPERATURE PROPERTIES OF AMORPHOUS AND GLASSY MATERIALS

D. D. Osheroff, Department of Physics
(415) 723-4228 02-2 $112,000

The low temperature dielectric properties of amorphous systems are being investigated. Convincing evidence has now been obtained that interactions between thermally active defects in glasses leads to a hole in the defect density at zero field similar to that observed in spin glasses. The importance of the implications of this hole for other low temperature properties will now be studied in the expectation that a better overall understanding of amorphous materials will result. Development of glass capacitance thermometry will continue incorporating adjustments for the complications implied by the more complex dielectric response due to the interactions of the defects.

461. HIGH RESOLUTION SPIN- AND ANGLE-RESOLVED PHOTOEMISSION FACILITY FOR HIGHLY CORRELATED ELECTRON SYSTEMS AT THE ADVANCED LIGHT SOURCE

Z.-X. Shen, Department of Applied Physics
(415) 725-8254 02-2 $300,000 (0 months)

Development of an experimental station at the Advanced Light Source for angle- and spin-resolved photoemission investigations of highly correlated electron systems.

462. SEARCH FOR THE MECHANISM OF HIGH TC SUPERCONDUCTIVITY

J. P. Collman, Department of Chemistry, 5080
(415) 725-0283

W. A. Little, Department of Physics
(415) 725-0283 03-1 $100,000

The proposed research is a two-pronged attack on the question of the nature of the mechanism responsible for the superconductivity of the high T_c superconductors using two newly developed techniques uniquely suited for such studies. One involves the measurement of minute changes in the reflectivity of a superconducting sample upon entering the superconducting state, and the other the use of tri-layer, N'NS proximity effect sandwiches for studies of interference phenomenon. Electrochemical experiments using the high T_c electrodes at cryogenic temperatures are also being conducted.

STATE UNIVERSITY OF NEW YORK AT BUFFALO
Buffalo, NY 14260-3000

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463. SUNY BEAMLINE FACILITIES AT THE NATIONAL SYNCHROTRON LIGHT SOURCE

P. Coppens, Department of Chemistry
(716) 645-2217 02-2 $250,000

Operation of beamline 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, E. I. DuPont de Nemours, Amoco Corporation, and collaborative work with numerous other institutions. The research interests are: structure of materials, electronic structure of materials, surface physics, compositional analysis, and time-resolved studies of dynamic processes.

464. X-RAY STUDIES OF MICROSTRUCTURES IN SEMICONDUCTOR AND SUPERCONDUCTING MATERIALS

Y. H. Kao, Department of Physics
(716) 645-2576 02-2 $100,000

State-of-the-art techniques making use of the high-intensity X-rays from synchrotron radiation are employed for a systematic study of the short-range-order microstructures in multilayer semiconductors. Emphasis on studies of semiconductor heterostructures and superlattices grown by molecular beam epitaxy. Focus is on the interfacial microstructures and the effects of chemical doping.

STATE UNIVERSITY OF NEW YORK AT STONY BROOK
Stony Brook, NY 11794-3400

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465. SELF-ASSEMBLY BEHAVIOR AND POLYMERIZATION PROCESSES IN SUPERCRITICAL FLUID COMPOSITES

B. Chu, Department of Chemistry
(516) 632-7928 03-2 $84,000

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

466. THE EFFECTS OF CONFINEMENT ON THIN POLYMER FILMS

M. Rafailovich, Department of Material Science
(516) 632-8483

J. Sokolov, Department of Material Science
(516) 632-8483 03-2 $60,000 (0 months)

This program studies the properties of homopolymers and block-copolymers confined to solid and liquid interfaces. The areas of research are the wetting of thin polymer films and polymer brushes, the dynamical properties of grafted polymers in melts and solutions, and the dynamics of asymmetric block co-polymer ordering near surfaces. Complementary experimental profiling techniques being used in this research include dynamic secondary ion mass spectroscopy (SIMS), atomic force and transmission electron microscopy (AFM and TEM), and neutron and X-ray reflectivity.

UNIVERSITY OF TENNESSEE
300 South College
Knoxville, TN 37996-1501

467. X-RAY SCATTERING FACILITY FOR DYNAMICS OF SURFACES AND INTERFACES

E. W. Plummer, Department of Physics & Astronomy
(423) 974-2288 02-2 $370,500

Design and construction of a bending magnet beamline and surface scattering endstation as BM9B at the Advanced Photon Source under the Complex Materials Collaborative Access Team (CMC-CAT). The first optics enclosure will be shared with a second beamline (for EXAFS and imaging). This is part of the sector operated by the Complex Materials Collaborative Access Team (CMC-CAT).

468. COMPOSITE FERMION APPROACH TO STRONGLY INTERACTING QUASI TWO DIMENSIONAL ELECTRON GAS SYSTEMS

J. J. Quinn, Department of Physics and Engineering Science and Mechanics
(423) 974-4089 03-2 $41,520

A composite Fermion approach is used to study the quasiparticle structure of a two dimensional electron gas in a magnetic field where the last Landau level is fractionally filled. The utility of an approximate hierarchical approach will first be verified and the utilized to study the quasiparticle excitations and interactions.

469. INVESTIGATIONS OF ISOTOPIC SUBSTITUTION, PRESSURE, POLYMER SEGMENT NUMBER AND DISTRIBUTION, ON MISCIBILITY IN POLYMER-SOLVENT AND POLYMER-POLYMER SYSTEMS

A. Van Hook, Department of Chemistry
(615) 974-5105 03-2 $112,500

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.

TEXAS A&M UNIVERSITY
416 Engin. Physics Bldg.
College Station, TX 77843

470. INFORMATION-BEARING STRUCTURES AND MAGNETISM OF THIN FILMS

V. Pokrovsky,
(409) 845-1175 02-3 $35,900

A theoretical investigation into the magnetic behavior of thin film ferromagnets will be performed to elluciate possible topological structures, their interactions, and their dynamics. Because the system both involves competition between weak interactions of exchange, spin anisotropy, and dipole-dipole magnetic coupling and also formally has no long range order (fluctuations are large), its behavior is very rich and quite sensitive to external perturbation. Structural types to be considered are Skyrmions, vortices, domain walls, and the glassy state. Applied magnetic fields and surface structure are the primary types of perturbing influences to be considered.

471. NOVEL BIOMATERIALS: GENETICALLY ENGINEERED PORES

H. Bayley,
(508) 842-9146 03-2 $181,104

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

UNIVERSITY OF UTAH
304 EMRO
Salt Lake City, UT 84112

472. THEORETICAL AND EXPERIMENTAL STUDY OF ORDERING IN III/V SYSTEMS

G.B. Stringfellow, Department of Materials Science and Engineering
(801) 581-8387 01-1 $114,650

Explore the kinetic processes leading to atomic scale ordering in III/V semiconducting alloys during epitaxial growth by organometallic vapor phase epitaxy (OVMPE). Emphasis on expanding the ordered structure domain size and increasing the degree of ordering. Characterization of the structural, electrical and optical properties by atomic force microscopy, high resolution electron microscopy, electron microprobe, X-ray diffraction, photoluminescence, optical absorption, and Raman spectroscopy. Materials for study include alloys of GaInP, GaInSb, GaSb, InPSb, and InAsSb.

473. OXIDE PEROVSKITES AS PROTONIC CONDUCTORS: THERMODYNAMIC STABILITY AND PROTONIC CONDUCTIVITY

A.V. Virkar, Department of Materials Science and Engineering
(801) 581-5396 01-3 $96,000

Thermodynamic stability of alkaline earth perovskites which are potential protonic conductors will be determined with respect to decomposition by H_20 and $C0_2$. Rare-earth (RE) doped $BaPr0_3$, $BaTh0_3$, and $Ba_3(CaNb_2)0_9$ will be investigated. Thermodynamic stability will be investigated by galvanostatic technique and by a molten salt method. Stability also will be tested in H_20 and $C0_2$ atmospheres. Thermogravimetry will be used to measure the incorporation of H_20. Conductivity will be measured by a complex impedance technique.

474. PROPOSAL FOR THE CONTINUATION OF THE PROGRAM ON THE SYNTHESIS OF MOLECULE/POLYMER-BASED MAGNETIC MATERIALS

J. S. Miller, Department of Chemistry
(801) 585-5455 03-1 $100,000

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

475. TRANSIENT AND CW OPTICAL STUDIES OF CONDUCTING POLYMERS

Z. V. Vardeny, Department of Physics
(801) 581-8372 03-2 $137,000

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

VIRGINIA COMMONWEALTH UNIVERSITY
Richmond, VA 23284-2000

476. CLUSTERS AND CLUSTER ASSEMBLIES
P. Jena, Physics Department
(804) 828-8991

B. K. Rao
(804) 828-1820

S. N. Khanna
(804) 828-1612 01-3 $183,936

Theoretical studies of the equilibrium geometries, electronic structure, stability, and reactivity of transition metal clusters using molecular orbital theory and molecular dynamics. Mobility of clusters on metal substrates. Design of stable clusters and energy band structure of cluster assembled crystals.

UNIVERSITY OF VIRGINIA
205 McCormick Road
Charlottesville, VA 22901

477. SUPERCONDUCTING MATERIALS
J. Ruvalds, Physics Department
(804) 924-6796 02-3 $55,000

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 anomalous damping observed experimentally and calculated by the principal investigator. Normal state properties of the high temperature oxides will be investigated, including i.e., reflectively, the Hall effect, electronic Raman scattering, and anomalous susceptibility.

WASHINGTON STATE UNIVERSITY
Pullman, WA 99164-2920

478. COARSENING IN MULTICOMPONENT MULTIPHASE SYSTEMS
J.J. Hoyt, Department of Mechanical and Materials Engineering
(509) 335-8523 01-1 $42,417

Theoretical and numerical analysis to extend recent methods of treating precipitate coarsening to systems that contain multiple components and more than one coarsening precipitate phase. The results, in addition to scientific value, may be of practical value in the design and optimization of new materials.

479. THE ROLE OF DEFECT STRUCTURES IN GRAIN BOUNDARIES ON THE DEFORMATION AND FRACTURE BEHAVIOR OF CRYSTALLINE SOLIDS
R.G. Hoagland, Department of Mechanical and Materials Engineering
(509) 335-8280 01-2 $98,248

In-situ TEM observations of gallium penetration along grain boundaries in aluminum. Impurity mobility in polycrystals, bi- and tri-crystals. Atomistic calculations of grain boundary defect structures via EAM. Correlation of Ga mobility and grain boundary structure.

WASHINGTON UNIVERSITY
One Brookings Drive
St. Louis, MO 63130-4899

480. QUANTUM-MECHANICALLY BASED INTERATOMIC FORCES AND MECHANICAL PROPERTIES OF MATERIALS
A. E. Carlsson, Department of Physics
(314) 935-5739 02-3 $30,000

Development of computation methods for calculation of interatomic potentials used in simplified tight-binding models of transition metals and their alloys. Extension beyond the tight-binding model. Interatomic potentials tested both by experimental data and density-of-states band calculations. Applied to surfaces and vacancies and subsequently used to calculate phase diagrams and the properties of dislocations and grain boundaries.

UNIVERSITY OF WASHINGTON
Box 351560
Seattle, WA 98195

481. X-RAY AND GAMMA-RAY SPECTROSCOPY OF SOLIDS UNDER PRESSURE

R. L. Ingalls, Physics Department
(206) 543-2778 02-2 $119,000

The structure and properties of materials are investigated using X-ray and gamma-ray spectroscopy. Emphasis is on materials undergoing pressure-induced phase transitions such as the B1-B2 crystal structure transition in alkali halides, the bcc-hcp transition in iron, rotational transition in rhenium trioxide, and the crystalline-amorphous transition in tin tetraiodide. Mossbauer studies are aimed at diamond anvil experiments with iron and its compounds that are of geophysical significance.

482. GROWTH AND PROPERTIES OF SILICON/FLUORITE HETEROSTRUCTURES

M. A. Olmstead, Department of Physics
(206) 685-3031 02-2 $38,000 (5 months)

Experimental investigation of the nucleation and growth of silicon on fluorite substrates, and on the investigation of the unique properties of the resultant interfaces and heterostructures. Goals are to control the formation of flat layers or compact islands, to determine the properties of oriented, crystalline silicon nanostructures surrounded by fluorite and/or vacuum, and to build a theoretical and experimental framework for heteroepitaxial systems involving strongly dissimilar materials.

483. SPIN DEPENDENT X-RAY SPECTROSCOPY THEORY

J. J. Rehr, Department of Physics
(206) 543-8593 02-2 $58,722

A theoretical-calculational investigation of various deep core X-ray spectroscopies such as X-ray absorption fine structure (XAFS), photoelectron diffraction (PD), and diffraction anomalous fine structure (DAFS). Development, maintenance, and distribution of computer codes to provide a state-of-the-art means to obtain a theoretical mimicry which can be compared with experimental XAFS-type spectra. Important features of the codes are portability and their ease of application to various X-ray spectroscopies. All relevant multiple-scattering and atomic vibrations effects are included in the codes. Special emphasis placed on the theoretical development of improved treatment of many-body and electron self-energy effects with their eventual inclusion into the library of codes, which is important in order to obtain the best possible agreement between calculated and experimental spectra in their near-edge region (less than 100 eV).

484. FURTHER XAFS INVESTIGATION OF PHASE TRANSITIONS

E. A. Stern, Department of Physics
(206) 543-2023 02-2 $80,000

Use of X-ray absorption spectroscopy to investigate phase transitions invarious materials. Investigation of lattice instabilities, defect structures, local deviations from average structure, and the range of interactions that cause structural instabilities. Examples of specific investigations are the range of the tetragonal distortion interaction in$PbTiO_3$, the antiferrodistortive transition in $Na_{1-x}K_xT_2O_3$, the orthorhombic to tetragonal transition in the high temperature superconductor $La_{2-x}Sr_xCuO_4$, and the local disorder in the $AgBr_{1-x}Cl_1$ system.

485. COMPLETION OF PACIFIC NORTHWEST CONSORTIUM FACILITIES AT THE ADVANCED PHOTON SOURCE

E. A. Stern, Physics Department
(206) 543-2023 02-2 $900,000

Completion of the development of Sector 20 by the Pacific Northwest Consortium-Collaborative Access Team (PNC-CAT) at the Advanced Photon Source. Included is the instrumentation of a facility for handling radioactive materials together with the necessary safety protocols to measure small volumes of radioactive samples. The research to be performed by the PNC-CAT will include investigations of the interaction of X-rays with matter, the development of new X-ray techniques and the application of these new techniques and others to the understanding of the basic properties of matter. A major focus is to use X-ray techniques to understand environmental science on a molecular basis to develop the knowledge and understanding needed to address important environmental problems.

UNIVERSITY OF WISCONSIN AT MILWAUKEE
Milwaukee, WI 53201

486. INELASTIC ELECTRON SCATTERING FROM SURFACES

S. Y. Tong, Department of Physics
(414) 229-5056 02-3 $89,961

Theoretical investigation of the geometric and dynamical properties of surfaces by use of ab initio multiple scattering methods to extract quantitative surface information from state-of-the-art experimental techniques. Exploration of electron and positron diffraction for surface structural studies using a combination of elastic scattering and emission techniques, as well as imaging techniques based on holographic principles. Interpretation of electron-phonon loss spectra to study localized excitations at metal-semiconductor interfaces and ultrathin epitaxial metal layers by use of highly precise first-principles models and inelastic multiple scattering theory. Some studies which deal with the relation between atomic structure and surface magnetism. Close collaboration with experimental programs based at universities and at DOE laboratories.

UNIVERSITY OF WISCONSIN
3731 Schneider Drive
Stoughton, WI 53589

487. SCANNING PHOTOEMISSION MICROSCOPY AT THE ALS

F. Cerrina, Center for Xray Lithography
(608) 877-2402 02-2 $32,000 (6 months)

Spatially Resolved Photoemission Spectroscopy with a probe beam of soft X-rays will be perfomed with a spot size very near the diffraction limit (<500A). This spectromicroscopy instrument, named MAXIMUM, will enable a careful examination of patterned or structured surfaces to determine local chemical and electrical properties. MAXIMUM, having demonstrated capability at Aladdin and on borrowed beamlines at the Advanced Light Source, will be moved to the interferometry beam line (12.0). Research topics will include electronic structure of non-ideal semiconductor surfaces; electronic states and local chemistry of semiconductor interfaces; polarization resolved (for either contrast or magnetization studies) microscopy; surface charges in highly insulating systems; failure mechanisms (electromigration and corrosion) of integrated circuit interconnects; solid state reactions in constrained systems (semiconductor silicides); local chemistry of Si and Si:Ge surfaces; and diamond film work function studies.

UNIVERSITY OF WYOMING
Laramie, WY 82071-3355

488. THE WYOMING DOE/EPSCOR PROGRAM

J.W. Steadman,
(307) 766-2240 05-1 $730,000

Fossil Energy, the efficient utilization of electrical energy, and environmental remediation and waste reduction are the focus research areas of the Wyoming DOE/EPSCoR project. The work of the fossil energy research cluster includes: studying CO_2 upgrading processes to reduce the moisture content of coal, understanding the critical role of air in the manufacture of formed-coke briquettes, addressing the problems associated with NO_x removal in coals, and focusing on hydrocarbon cracking and reforming operations in the petrochemical industry. The second research team, studying the efficient utilization of electrical energy, is developing methods for detecting and correcting degradations in systems driven by motors, measuring and understanding the radio frequency interference created by modern high-efficiency invertors, and integrating photovoltaic energy sources into power distribution grids. The environmental remediation and waste reduction project involves studies of rhizosphere microbial communities to extract metal contaminants from soils and the elimination of volatile organic carbon emissions during the dehydration of natural gas.

SECTION C

Small Business Innovation Research

ADHERENT TECHNOLOGIES, INC.
9621 Camino del Sol NE
Albuquerque, NM 87111-1522

489. ULTRAFAST POLYSILYLENE SCINTILLATORS
L. A. Harrah,
(505) 822-9186 PH-2 $124,249

Scintilator fluors with short radiative decay times are sought for a variety of reasons including: Operation at higher counting rates and resolving fast radiation events; Polymers that have delocalized first electronic excited states, and consequently rapid decay, are studied as scintillator fluors. Fluors with both high quantum yields and very short decay times were identified in this effort; estimated decay times of less than 300 picoseconds and fluorescence quantum yield, spectra and energy transfer from common scintillator hosts. Light yields were compared with slower scintillator fluors indicating similar results, but with potentially much faster response. Fluorescence lifetimes were estimated based on a model of their behavior. In Phase II, fluorescence lifetimes will be measured and structures synthesized and optimized for yield and rapid decay time. New host materials will also be investigated that have higher mean atomic number with the attendant increase in photoelectric effect energy deposition rather than the Compton scattering deposition typical of low Z (atomic number) materials in organic hosts. While high Z liquids will be a primary goal, solid host materials that can be formed into good optical quality, large volume shapes will also be sought.

ADVANCED MATERIALS CORPORATION
700 Tech. Drive, PO2950
Pittsburgh, PA 15230-2950

490. A SIMPLE PROCESS TO MANUFACTURE GRAIN ALIGNED PERMANENT MAGNETS
V. K. Chandhok,
(412) 268-5649 PH-1 $74,840

Traditional methods for manufacturing of high energy anistropic permanent magnets require many processing steps such as pulverizing, milling, grain alignment, cold compaction, and sintering. Development of a simpler process that creates a grain aligned structure will significantly reduce the cost of high energy permanent magnets. Attempts will be made to fabricate grain oriented permanent magnets with the proposed single step process. Crucial processing elements will be carefully evaluated to determine if high performance magnets can be fabricated with this method. The proposed process is generally applicable to any magnet material with crystalline anisotropy but perhaps with different degrees of success. During Phase I test runs will be made for neodymium-iron-boron based material. If successful, process optimization and ncessary work for the development of industrial process will be performed during Phase II.

491. A NOVEL TECHNIQUE FOR THE ENHANCEMENT OF COERCIVITY IN HIGH ENERGY PERMANENT MAGNETS
S. G. Sankar,
(412) 268-5649 PH-1 $73,130

Permanent magnets with energy products greater than 50 MGOe have been realized in the laboratory for neodymium-iron-boron, but they do not possess sufficiently high coercivity to allow reliable operation of electromechanical devices. Improvement in the coercivity requires the control of the type and amount of the intergranular phases and the judicious substitution of heavy rare earth atoms into the intergranular phase. These issues will be addressed by utilizing a new processing method which we have recently devised. We propose a process of intergranular phase control and selective atomic substitutions into the intergranular phase with an objective to produce magnets with energy products of ~55 MGOe and an intrinsic coercivity of >15 kOe.

ADVANCED REFRACTORY TECHNOLOGIES, INC.
699 Hertel Avenue
Buffalo, NY 14207-2396

492. DIAMOND-LIKE NANOCOMPOSITES: HARD, WEAR RESISTANT, LOW FRICTION COATINGS FOR TRIBOLOGICAL APPLICATIONS
D. Kester, Sr.,
(716) 875-4091 PH-1 $74,869

Novel thin film coating materials with high hardness levels are being sought for tribological applications. A new class of thin film coating materials, diamond-like nanocomposites (DLN), have been developed which have the properties of high hardness, low wear, and low friction. They are amorphous, very smooth, and have excellence adhesion to most substrate materials. They have specific advantageous over similar, competing technologies such as diamond and diamond-like carbon thin films, including having stress levels which are much lower at equivalent hardness levels. In Phase I of this program we propose to maximize the hardness of the coatings through varying the deposition parameters and process. Work will also be performed on optimizing the properties of war performance, friction, and adhesion and on understanding how deposition conditions affect each of these properties. The coating-substrate interface will be studied to determine how it influences tribological performance.

ADVANCED TECHNOLOGY CORPORATION
661 Emory Valley Road
Oak Ridge, TN 37830

493. NONDESTRUCTIVE MEASUREMENTS OF KEY MECHANICAL PROPERTIES OF ALLOY 718 WELDED STRUCTURES USING NOVEL STREE-STRAIN MICROPORBE TECHNOLOGY

F. M. Haggag,
(423) 483-5756 PH-1 $75,000

This project proposes to utilize the newly developed stress-strain microprobe (SSM) to characterize condition of nickel-based alloy 718 welds following various thermal treatments which resulted in the deterioration of their mechanical and fracture properties. The automated ball indentation (ABI) technique of the SSM system has recently been shown to yield indentation energy to fracture (IEF) from the indentation load versus depth curves. The IEF values (calculated from the measured ABI load-depth curves at various test temperatures and using critical fracture stress and strain models) were successfully correlated to the conventionally-measured fracture toughness of several nuclear pressure vessel steels. Since ABI is essentially nondestructive, the technique could be used periodically to evaluate and monitor the condition of the structures in-service to assure integrity and safety, as well as to avoid premature decommissioning. In materials such as alloy 718, which are sensitive to the chemical composition and thermal-mechanical processing, correlations should be established beween their microstructure and ABI measurements before the technique can be applied for damage characterization and remaining life prediction. We propose to establish these correlations by a detailed characterization of the microstructures of as fabricated and aged alloy 718 welds and their ABI parameters. Fortunately, the ABI technique requires minimal specimen preparation and coupons used for scanning electron and optical microscopy can be used for ABI tests as well. Phase II addresses extensions of these correlations to characterization of the property changes of alloy 718 welds in-service and the development of a portable (robotic) probe system for testing structures in various plants.

APPLIED SCIENCE AND TECHNOLOGY, INC.
35 Cabot Road
Woburn, MA 01801-1053

494. HIGH GROWTH RATE CUBIC BORON NITRIDE DEPOSITION

R. Gat,
(617) 933-5560 PH-1 $74,867

Cubic Boron Nitride (cBN) is an excellent machine tool material and tribological coating because of its hardness (greater than 60Gpa). Current low pressure deposition technology of cBN produces highly stressed films containing only fractional volume of cBN that is deposited at very low rates. We propose to develop a high rate cBN deposition process using microwave plasma. A new high density fully ionized B+ and N+ plasma sputtering source with independently controllable target and substrate ion energy will be used. Selective etching of non-cubic BN will be evaluated as a means for improved film crystallinity.

APS MATERIAL, INC.
4011 Riverside Drive
Dayton, OH 45405

495. CONTROLLED ATMOSPHERE PLASMA SPRAYING OF NDFEB MAGNET MATERIALS

M. C. Willson,
(937) 278-6547 PH-1 $75,000

There is a need for new permanent magnet processing methods to improve the intrinsic coercivity of NdFeB and other rare-earth materials. Many applications, such as permanent magnet motors, utilize thin magnet shapes that operate under high demagnitizing conditions requiring high coercivity. The controlled atmosphere plasma spray process has the potential to achieve high coercivity in both a near shape and processed NdFeB particulate form. The proposed Phase I project will determine the feasibility of this process to produce high coercivity magnet materials. Success in the Phase I project would then lead to a scale up of the process in Phase II to produce larger volumes of high coercivity NdFeB material in near net shape or particulate form in an economically competitive manner with existing permanent magnet manufacturing methods. APS Materials, Inc., in conjunction with the University of Dayton Research Institute Magnet Laboratory, will investigate the ability of the controlled atmosphere plasma spray process to fabricate NdFeB magnets with acceptable magnetic properties. The initial work will concentrate on optimization of process variables as they affect the coercivity and other properties of NdFeB material. Magnet alloy feedstock composition, particle size, and chamber atmosphere will be investigated to further optimize the final processed product. Both material and magnetic properties of the processed NdFeB will be measured during the course of the project.

ARACOR
425 Lakeside Drive
Sunnyvale, CA 94086-4704

496. HIGH GAIN MONOCAPILLARY OPTICS

E. D. Franco,
(408) 733-7780 PH-2 $280,047

Glass capillaries, with tapered geometries and narrow exit apertures, have demonstrated substantial improvements to the flux of 1 to 20 keV X-rays which can be funneled into micron scale beams. The main barrier to their useful deployment on both synchrotron and laboratory X-ray instruments has been the lack of a reproducible and well-controlled fabrication technique. This problem will be addressed through the development of a next-generation capillary puller for elliptical, parabolic, and conical capillary designs. The overall objective of this project is to improve control over the fabrication process so that capillary optics can be reliably produced with gains greater than a factor of 100 over what can be achieved with pinhole collimation. In Phase I we instrumented the draw tower with sensors to measure the position and shape of the capillaries and the temperature profile of the furnace. This diagnostic capability allowed us to develop a reproducible technique for producing conical capillaries with an exit diameter of less than 2 um. These same diagnostic techniques allowed us to identify sources of mechanical instabilities that lead to flaws in the figure and linearity of the capillary optic. In Phase II, we will correct these instabilities, develop techniques for fabricating elliptical, parabolic, and conical capillaries, and explore laboratory and synchrotron analytical applications made possible by these optics.

CHEMAT TECHNOLOGY, INC.
19365 Business Center Dri
Northridge, CA 91324

497. STABILIZATION OF NITRIDE PERMANENT MAGNET MATERIAL VIA SOL-GEL ROUTE

Y. Huang,
(818) 727-9786 PH-1 $75,000

The discovery of Nd-Fe-B and R_2Fe_{17} nitride magnetic materials had drastically initiated a worldwide search and impact the market due to their magnetic properties and cost effective. $Sm_2Fe1_7N_x$, has comparable saturation magnetization, higher T_c, anisotropy field and coercivity to that of Nd-Fe-B. However, commercialization of this material, two major problems need to be solved:
(1) Sm_2Fe_{17} nitride decomposes to Sm nitride and iron when heating to temperature above about 600°C, which prohibits application of this material as sintered magnets using current technologies. The application is limited in bonded magnets, (2) Degradation of magnetic properties of this material with time, which is coincided related to current used processing technologies. There is a need of revolutionary technology reform to realize the superior magnetic properties of R_2Fe_{17} nitride materials. We propose to fabricate rare-earth+Fe intermetallic nitride through sol-gel route. Sol-gel technology is chosen because of a variety of advantages, including excellent control of stoichiometry of precursor solutions, directly fabrication of nitride, low sintering temperature, homogeneity of the materials and fine grain structure, low cost, and simple and inexpensive equipment. Nitride powders and sintered magnets can be fabricated at low temperature and no further nitrogenation is needed.

ELTRON RESEARCH, INC.
5660 Airport Blvd., #105
Boulder, CO 80301-2340

498. ADVANCED MULTILAYER BRAZE FOIL FOR SI_3N_4 JOINING

W. J. Donahue,
(303) 440-8008 PH-1 $74,997

Si_3N_4 is an important light weight structural ceramic due to its hardness, wear resistance, high temperature oxidation resistance and strength. However, the exploitation of its superior mechanical and chemical properties depends upon reliable joints that can withstand high temperature corrosive environments. Presently, the use of advanced ceramics in critical applications is limited by a lack of an economical technique for effectively joining these materials. This program will study layered Cr/CrN/Ni-Cr-Si/CrN/Cr foils for use in Si3N4 brazing applications. Ni-Cr foils have serveral attractive characteristics, including good $S_{i3}N_4$ surface wetting, high temperature strength and oxidation resistance. A high activity Ni-Cr alloy braze incorporating approximately 10% silicon, will be used to create a strong joining interaction where the formation of brittle silicides and porous microstructures are limited by a predeposited CrN diffusion layer. Chromium will act as a surface treatment to ensure uniform ceramic-braze interfaces and good wetting across the joint interface. The sophisticated chemistry found in this joining issue will be addressed in a prefrabricated multilayer braze foil product. The foil will be easily handled and applied to the joint interface. Successful completion of this program will lead to the development of a strong A(>400MPa at 900°C) and reliable (high Weibull Modulus) Si_3N_4-Si_3N_4 and Si_3N_4-metal joining technique. This Phase I project will address the fabrication of multilayer foils with various layer thicknesses to determine the relationships between foil layer thicknesses, brazing times, reaction product distributions and microstructure within the joint region, and joint strengths.

FORMCAST, INC.
14515 W. Cedar Avenue
Denver, CO 80223

499. DEVELOPMENT OF ECONOMICAL PROCEDURES FOR PRODUCING AND PROCESSING FINE GRAINED SSM FEEDSTOCK VIA MECHANICAL STIRRING

N. H. Nicholas,
(303) 778-6566 PH-1 $72,667

Semisolid metal (SSM) forming to near net shape of Al alloys for automotive, aerospace and military applications requires a fine grained, spheroidal primary solid feedstock for subsequent reheating and forming. Small diameter feedstock represents a significant segment of the SSM forming market. Magnetohydrodynamic stiring/direct chill continuous casting and wrought processing are current commercial routes to the repoduction of large and small diameter feedstock, respectively. Both routes are uneconomical. Magnetohydrodynamic stirring for feedstock is energy intensive and wrought processing routes to feedstock are energy and processing intensive. A more economical processing route to fine grained feedstock is required. In addition, magnetohydrodynamic stirring/direct chill continuous casting of feedstock, with coupling of slurry production and solidification, results in a rheologically deleterious surface dendritic microstructure that would be a significant problem in forming small diameter feedstock and must be dealt with in forming large diameter feedstock.

FRONT EDGE TECHNOLOGY, INC.
13455 Brooks Drive
Baldwin Park, CA 91706

500. DEVELOPMENT OF NOVEL, BORON-BASED MULTILAYER THIN FILM

S. K.-W. Nieh,
(818) 856-8979 PH-1 $73,420

The objective of this proposal is to develop a novel, superhard, boron-based, multilayer coating for various tribological applications. Boron-based coatings have been known for their extreme hardness. The best known example is the Ti-B-C-N system, with its hardness reaching 7,200 kgf/mm^2, which is between diamond and c-BN. In this proposed research, a continuous-feed in-line plasma enhanced sputtering process will be used to deposit a boron-based graded multilayer coating on metal and ceramic substrates for tribological applications. This graded multilayer coating will be comprised of a very thin metal adhesion layer (for its good adhesion to substrates), a transitional Ti-B layer, and a top superhard Ti-B-C-N layer. The thickness of each individual layer will be adjusted for tailoring of the coating properties and performance. The advantages of this graded multilayer coating include good adhesion to the substrate, high toughness, and most importantly, extreme hardness. The microstructure, mechanical properties and tribological behavior of this graded multilayer coating will be fully characterized. The optimum coating conditions and structure to achieve the best trbiological properties will also be developed. Furthermore, the low-cost advantage of using FRONT EDGE's continuous-feed, in-line, plasma enhanced sputtering system will also be clearly demonstrated.

GOSS ENGINEERS, INC.
3525 South Tamarac Drive
Denver, CO 80237

501. SHAFT WELD REPLACEMENT WITH A CERAMIC LOCKING ASSEMBLY JOINT

J. L. Gross,
(303) 721-8783 PH-1 $74,986

This proposal develops an innovative and highly efficient joint technology for the replacement of welded joints in shafts to mill heads. A common shaft failure is caused by the welding of the mill head to the shaft. Our innovative concept involves the novel use of machinable ceramics and locking assembly joints that will eliminate the current welding methods and maintain the structural intregity of the mill head and the shaft while providing improved heat insulating characteristics. The new joint technology can be manufactured economically with current manufacturing capabilities. Finite Element Stress Analysis and heat transfer analysis models will be used to examine the significance of several engineering development areas and to optimize the future of ceramic-metal shaft to mill head joining technology.

GREEN DEVELOPMENT, LLC
16164 West 13th Place
Golden, CO 80401-2983

502. DEVELOPMENT OF OPTIMAL SNO_2 CONTACTS FOR CDTE PHOTOVOLTAIC APPLICATIONS
J. Xi,
(303) 278-4571 PH-2 $750,000

We are proposed to extend the research and development to the following areas: 1. further optimization of the SnO_2 (F) deposition parameters; 2. exploration of APCVD growth of alternative TCOs that exhibit lower sheet resistance, higher optical transmission, and a smoother texture than SnO_2 (F); 3. development and optimization of diffusion barrier oxide layers by atmospheric pressure chemical vapor deposition method; 4. development of a low-cost, prototype, large-area atmospheric pressure chemical vapor deposition system.

HIRSCH SCIENTIFIC
365 Talbot Ave., Suite D8
Pacifica, CA 94044-2634

503. HIGH PERFORMANCE X-RAY AND NEUTRON MICROFOCUSING OPTICS
G. Hirsch,
(415) 359-3920 PH-2 $86,250

The use of extremely small diameter X-ray beams is expected to become an important experimental technique for researchers in materials science, biology, medicine, microelectronics, and many other scientific disciplines. While tapered glass-monocapillary optics have recently been developed to produce these microbeams, several technical issues have prevented this technology from achieving its full potential. First, it is difficult to produce capillaries having ideal taper profiles, extremely straight bores, and exceedingly low surface roughness. Secondly, the selection of materials suitable for fabricating the devices using conventional methods is narrow. This project is investigating an innovative approach for generating optics possessing optimized capillary shapes, in addition to allowing wide latitude in the material choice for the capillary interior. This will allow the highest possible microfocusing efficiency to be obtained for X-rays, as well as neutrons. Phase I research was successful in establishing the feasibility of the proposed fabrication method. A process for producing short capillary segments having extremely smooth gold reflecting-surfaces, along with well controlled taper profiles was demonstrated. Direct X-ray testing with synchrotron radiation verified the high reflectivity of the capillary material. Phase II research will continue this program with the goal of producing full size, high-performance microfocusing devices. These optics will be tested using several different radiation sources.

HOT METAL MODLING, INC.
35 McClellan Blvd.
Arkadelphia, AR 71923-8809

504. SEMI-SOLID THERMAL TRANSFORMATION TO PRODUCE SEMI-SOLID FORMABLY ALLOYS
J. R. Sarazin,
(501) 245-2513 PH-1 $750,000

Semi-solid forming is a process by which alloys are heated into a temperature range in which both liquid and solid phases are present. In this case, there is potentital for relatively easy casting or forging. This is largely due to a significant volume fraction of liquid phase. This has been traditionally accomplished by electromagnetic or mechanical stirring of the liquid slurry or semi-solid. This "breaks-up" the dendritic structure evident in a conventionally solidified ingot. The cost of the preparation of semi-solid alloys is relatively high due to expense associated with electromagnetic or mechanical stirring of the liquid alloy. The principal objective of this Phase I proposal is to develop new, less expensive, energy efficient processes for producing alloys that can be heated into the semi-solid temperature regime with a spheroidized substructure that will allow effective formability. All manufacturers of semi-solid alloys currently utilize electromagnetic or mechanical stirring to produce the spheroidized. Phase I will utilize air-slip direct-chill-cst A356 and 357 ingots to heat to specific temperatures and times using new instrumentation to produce formable semi-solids alloys.

HYPER-THERM HIGH-TEMPERATURE COMPOSITES, INC.
18411 Gothard St., Unit B
Huntington Beach, CA 92648-1208

505. NANO-LAYERED DIBORIDE MATERIALS WITH ENHANCED HARDNESS, STRENGTH, AND TOUGHNESS FOR WEAR APPLICATIONS

R. J. Shinavski,
(714) 375-4085 PH-1 $74,929

Many of the superhard (>30 GPa) ceramic materials have not been utilized to the extent expected in wear applications. The promise of these materials is based on their hardness being higher than materials conventionally selected, particularly for material transfer applications subjected to erosive wear. This lack of market penetration is due to the absence of adequate strength, and failure during use. This "brittleness" is intrinsically linked to their strongly bonded covalent nature that results in their attractive hardness properties. However, the possibility of engineering the desired properties into the material through the additions of a second phase are promising. Recent research has suggested that nano-layering of materials can result in dramatically enhanced values of hardness and strength when at least one of the constituent layers is on the order of 10 nm thick. This work will investigate the degree and presence of these nanolayering enhancements in a superhard diboride nanolayered system. Diboride nanolayer compositions have been selected that are predicted to result in a significantly tougher material, while maintaining the high hardness characteristics; or to maximize hardness of the nanolayered structure. The nanolayered materials will be produced via chemical vapor deposition (CVD). This approach is the most commercially viable method for producing nanolayer coatings due to the excellent process control and adaptability to coating various geometries and large numbers of components. The nanolayered materials will be investigated microstructurally and mechanically in order to establish the structure-property relationship of the nanolayering effect. This Phase I work will identify nanolayered diboride compositions from which coated wear components can be fabricated for slurry pumps or cutting tools.

INTERNATIONAL SOLAR ELECTRIC TECHNOLOGY
8635 Aviation Blvd.
Inglewood, CA 90301-2001

506. LARGE AREA, LOW COST PROCESSING FOR CIS PHOTOVOLTAICS

B. Basol,
(310) 216-4427 PH-2 $750,000

CIS and related compound semiconductors are important photovoltaic materials. Although CIS devices are the highest efficiency thin-film solar cells ever produced, they are not commercially available because of difficulties associated with the costly processing schemes employed in the fabrication of these devices. The purpose of the proposed work is to develop and demonstrate a lower cost, more robust, large area processing techniques for CIS photovoltaics. During Phase II of this project, 1 ft^2 area CIGS thin film photovoltaic modules will be developed with conversion efficiency of 10%.

ISM TECHNOLOGIES, INC.
9965 Carroll Canyon Road
San Diego, CA 92131

507. ADVANCED PLASMA SURFACE MODIFICATION SYSTEM

J. R. Treglio,
(619) 530-2332 PH-1 $74,669

A. Systems are not commercially available that can surface treat large areas of both metals and non-conductors efficiently. In particular, systems that can ion implant and/or deposit hard coatings using the most advanced processes do not exist. B. ISM proposes to address this problem by combining its advanced vacuum arc multiple metal ion source technology with an array of plasma deposition sources, forming a system wherein all steps in a process -- sputter cleaning, ion implantation, and coating -- can take place in a single chamber. C. In Phase I, the general concept will be tested using ISM's small, in-house single source implanter with a focused cathodic arc source. D. In Phase II, ISM's multisource metal ion implanter will be combined with multiple cathodic arc sources to demonstrate full commercial-scale surface treatment.

MATERIALS & ELECTROCHEMICAL RESEARCH (MER) CORPORATION
7960 South Kolb Road
Tucson, AZ 85706

508. A NOVEL TECHNOLOGY FOR SI_3N_4-TO-SUPERALLOY JOINTS WITH HIGH USE TEMPERATURE CAPABILITY

S. Guha,
(520) 574-1980 PH-1 $75,000

Advanced heat engines require joints between high temperature ceramics (Si_3N_4, SiC) and metal alloys (Inconel 718 or Incoloy 909) with use temperature capabilities in the range 650-900°C. The joining problem is complicated due to the residual stresses generated within the ceramic that arise from the mismatch in thermophysical properties between the ceramics and metals; frequently, the ceramic will crack as a result of these residual stresses. The state-of-the-art in joining technology is to join such ceramics to metals using soft metal interlayers (e.g. Cu or Ni). Unfortunately, the elevated temperature use capability for such joints is then severely limited due to the low strength of the soft interlayer at these use temperatures. A novel joining approach is proposed where the joint will be first designed to lower the residual stresses to the point that they permit direct bonding between the ceramic and the metal, followed by bonding them using metal interlayers that shield at low temperatures but retain their strength at elevated temperatures. This will allow the dissipation of stress at lower temperatures through plastic yielding without compromising the elevated temperature use capability. A unique stress modeling approach that has been developed at MER over the past three years will be used in the design of joints. The model allows for more quantitative estimates of residual stresses (e.g. a criterion that predicts whether a specific joint configuration will survive the post-brazing cool-down cycle or not). The joinint technology will be demonstrated for Si_3N_4-Incoloy 909 system.

NANO INSTRUMENTS, INC.
1001 Larson Drive
Oak Ridge, TN 37830

509. PROCESSING FOR SURFACE HARDNESS: NOVEL CHARACTERIZATION TECHNIQUES FOR DYNAMIC TRIBOLOGICAL PROPERTIES OF THIN FILMS

W. C. Oliver,
(423) 481-8454 PH-1 $74,993

The goal of this Phase I program is to address the issues and design criteria necessary to enable dynamic tribological testing to be performed at the nanoscale. Currently, there exists a broad range of applications for which the ability to produce an adherent, hard, thin, wear-resistant coating plays a critical role. The capacity to mechanically characterize these coatings is often paramount in evaluating their potential performance. Quasi-static tests, such as nanoindentation, are widely used to assess the quality of these thin hard coatings. However, as the thickness of the coatings decreases to less than 20 mm, the ability to characterize their properties using normal indentation techniques becomes increasingly difficult due to physical limitations of the indenter geometry. It is also known that normal indentation tests do not always correlate well with wear properties. Dynamic tribological properties at the nanoscale are, therefore, of interest. While no true nanoscale tribological systems exist, Nano Instruments has demonstrated the ability to perform nanoscale scratch experiments of a limited nature. While the extension of this current technology to more conventional wear experiments on the nanoscale is a challenging task, it is of vital importance to a variety of U.S. industries.

NANOMATERIALS RESEARCH CORPORATION
2849 East Elvira Road
Tucson, AZ 85706-7126

510. A NOVEL PROCESS TO PRODUCE NANOSTRUCTURED PERMANENT MAGNETIC MATERIALS

S. A. Pirzada,
(520) 294-7115 PH-1 $750,000

Permanent magnets are being used in a variety of consumer, industrial, and defense applications. With the discovery of rare-earth based magnet materials, the properties of permanent magnet devices have been improved substantially. This program aims at demonstrating and developing a cost-effective technology to produce nanostructured magnetic materials with improved magnetic properties. Nanomaterials Research Corporation (NRC) will, during Phase I, demonstrate the proof-of-concept that nanostructured magnetic materials with improved magnetic properties can be produced in bulk quantities at an affordable cost. Phase II will optimize the technology, while Phase III will commercialize it.

NANOPOWDER ENTERPRISES, INC.
120 Centennial Ave., Su B
Piscataway, NJ 08854-3908

511. A NEW SEMI-SOLID FORMING PROCESS FOR THE FABRICATION OF HIGH VOLUME FRACTION (>15 VO.%) METAL/METAL CARBIDE NANOCOMPOSITES

G. Skandan,
(908) 885-5909 PH-1 $750,000

We propose to develop a new method for semi-solid forming of high volume fraction (30-70 vol%) carbide containing alloys at a relatively low temperature (~1100°C). The process relies upon the formation of a low melting point multi-component liquid, containing a high volume fraction of nanostructured M_6C carbides. The size, morphology and volume fraction of the carbdes are controlled in the prealloyed powders, and therefore, no special methods are required to obtain a carbid/metal slurry with equiaxed grains, as is required in the case of conventional semi-solid forming methods. Preliminary experiments have demonstrated that it is possible to "mushy form" a 68 vol% M_6C carbide containing iron-base alloy at 1100°C. Since no dendritic phases are formed during our semi-solid forming process, expensive intermediate steps such as electromagnetic stirring are completely avoided. Furthermore, presently available die and tooling materials can be used to "mushy form" these materials. In Phase I, we will demonstrate the feasibility of forming simple symmetrical shapes from pre sintered powder compacts of iron-based alloys by making molds using ceramic materials (alumina), which will enable us to investigate the characteristics and reproducibility of the mushy formed parts for applications in automobile tooling (drills, reamers and dies), and automobile parts (bearings, cylinder liners, rocker arms, and valves). The process can be adapted to a variety of nickel- and cobalt-base alloys as well. In Phase II, the process will be optimized by careful selection of mold materials and alloy systems for desired end products for automotive and aerospace companies such as Pratt & Whitney, GE, McDonald Douglass, Carpenter Technology, Greenleaf Industries, and SKF Bearings.

OPTOMEC DESIGN COMPANY
13170B Central Ave, SE
Albuquerque, NM 87123-3032

512. ALTERNATIVE METAL FORMING USING LASER ENGINEERED NET SHAPING

D. M. Keicher,
(505) 343-9139 PH-1 $74,777

Laser Engineered Net Shaping is a solid freeform fabrication technology currently under development at Sandia National Laboratories for weapons applications. Sandia has demonstrated the ability of this process to produce near net shape stainless steel components with excellent material properties directly from computer-aided-design files. However, parts produced with this process currently have limitations due to inadequate surface finish and dimensional accuracy. Optomec's objective is to develop a laser-based process to re-melt the rough surface produced by the Laser Engineered Net Shaping process to improve surface finish and dimensional accuracy. This re-melt might be possible with the laser beam slightly defocused and moved in a random motion across the surface. Optomec proposes during Phase I, through its unique relationship with Sandia National Laboratories, to conduct a series of simple experiments to determine the feasibility of using laser-based techniques to improved surface finish and dimensional accuracy of parts produced with the Laser Engineered Net Shaping process. These simple experiments must necessarily precede Phase II fabrication of a Laser Engineered Net Shaping device incorporating laser-based re-melt capability.

PLASMAQUEST, INC.
850 North Dorothy Drive
Richardson, TX 75081-2769

513. HIGH-FLUX, LOW-ENERGY, ION SOURCE FOR HIGH RATE ION-ASSISTED DEPOSITION OF HARD COATINGS

C. Doughy,
(972) 680-1811 PH-1 $75,000

Many hard materials of potential industrial interest (e.g. cubic boron nitride) require high degrees of ion bombardment in order to produce acceptable films. We proposed to develop an ion source suitable for high rate deposition of hard coatings over large areas. Phase I will concentrate on demonstration of a plasma based ion source capable of generating a plasma density of 1011-1012/cm^3 over a 14 in. dia. The source will utilized a permanent magnet configuration to be developed under this grant, which results in low magnetic fields at the sample surface and enhance cross field diffusion. The source will be based on an electron cyclotron resonance (ECR) and will incorporate an integral sputter source for deposition. By coupling the high density plasma and integral sputter source, an industrially attractive source for deposition is created. Phase II will concentrate on deposition of films requiring a high degree of ion bombardment, e.g. cubic boron nitride, C_3N_4, diamondlike carbon.

SIENNA TECHNOLOGIES, INC.
9004 Inverness Drive NE
Seattle, WA 98115-3980

514. A NOVEL REACTIVE JOINING COMPUOND FOR HIGH TEMPERATURE APPLICATIONS

C. Toy,
(206) 528-5901 PH-1 $74,993

Currently available active brazing alloys are not suitable for high temperature applications. New brazing alloys and compounds are required to obtain reliable ceramic-to-ceramic and ceramic-to metal joints. In this project, a novel solid-state bonding approach is proposed to make SiC-SiC joints. Several compositions in the Ti-Si-C system will be investigated to develop a reliable reactive joining compound. The joining compound can also be used to repair cracks on SiC parts in the field. Phase I study will determine a reactive composition that can be applied with no external pressure and evaluate the mechanical properties of the joints. Mechanical properties, microstructures and microchemistry of the joints will be evaluated to select a final composition for a detailed Phase II study.

STIRLING TECHNOLOGIES, INC.
102 Walton Lane
Oak Ridge, TN 37830-8237

515. AN ION SOURCE DESIGN USEFUL FOR THE PRODUCTION OF TRIBOLOGICAL THIN FILMS

W. L. Stirling,
(423) 483-0142 PH-1 $74,996

This proposal addresses a need in industry for the generation of hard thin films with low energy ions of uniform flux over large areas. The need is similar to that for next generation etching requirements of 200 mm wafers with very small circuit dimensions (sub-microns) which are produced by a neutral stream of a halogen gas with energy in the range of 10 to 300 eV. The work outlined in this proposal will produce a design for an ion source concept that will be able to incorporate presently proved cleaning and thin film deposition methods with the ability to provide processing of both metal and insulating target substrates with either ion or neutral beams in the 20 to 200 eV range. The Phase I work will produce a source design based on techniques recently developed in controlled fusion research. The design will employ a unique ion acceleration scheme that is not space charge limited; beam blowup at the desired low energies will not be a problem. Also, the acceleration mechanism is easily scaled in size. Phase.II will affort a means of testing a full scale, prototype source of commercial interest.

SURMET CORPORATION
33 B. Street
Burlington, MA 01803

516. FABRICATION OF ACTIVE BRAZE ALLOYS FOR HIGH TEMPERATURE SERVICE

S. A. Sastri,
(617) 272-3250 PH-1 $75,000

The current impetus to develop high performance joining technologies stems from the anticipated use of advanced technical ceramics in structural applications that will exploit their desirable high temperature properties. Examples of such applications would include those for internal combustion engines, turbine engines and heat exchangers to mention a few. A simple yet flexible and broadly applicable innovative technique is proposed in Phase I as a way to fabricate and evaluate novel active braze alloy compositions that will meet these requirements. The expensive and time consuming conventional method of having to make ingots by melting, etc. will not be necessary. The technique is ideally suited for screening a whole series of new alloy compositions that would not normally be considered for the brazing of ceramics. The Phase I approach should be equally applicable to many types of ceramics including oxides such as alumina zirconia and non oxides such as silicon sarbide, silicon nitride and aluminum nitride ceramics. Once the technical feasibility is demonstrated in Phase I these broadly applicable and potentially low cost novel active braze alloy foils will face rapid development in Phase II and successful commercialization in Phase III.

UNISUN
587-F North Ventu Park Rd
Newbury Park, CA 91320-2723

517. IMPROVED PROCESSES FOR FORMING CIS FILMS

C. Eberspacher,
(805) 499-7840 PH-2 $750,000

This project is directed at a new technique for fabricating thin films of copper indium selenide (CIS) and its alloys for low-cost photovoltaic solar cells. Solar cells technologies based on CIS materials have achieved the highest sunlight-to-electricity conversion efficiencies of any polycrystalline thin-film photovoltaics (PV) technology, but CIS-based PV products have yet to be introduced in the commercial marketplace in large part due to the lack of simple, robust processes capable of depositing high-quality CIS films at low costs on large areas with the high-volume reproducibility needed for commercial production. This project is based on a simple, self-limiting, non-vacuum technique for fabricating CIS films for solar cells. The three basic steps are to form precursor materials, to deposit a film of these precursor materials, and to convert the precursor film to a CIS film. In Phase I we demonstrated that suitable precursor materials can be prepared; that precursor materials can be deposited as reasonably continuous, cohesive, adhesive precursor layers on suitable substrates; and that precursor films can be converted into reasonably dense, cohesive, adhesive CIS films believed suitable for solar cell fabrication. The key goals of Phase II will be to produce and/or procure increased quantitites of a variety of suitable precursors, to deposit uniform high-quality CIS films on large area substrates, to fabricate PV devices with state-of-the-art efficiencies, and to demonstrate the overall commercial potential of the technology.

SECTION D

DOE Center of Excellence for the Synthesis

and Processing of Advanced Materials

DOE CENTER OF EXCELLENCE FOR THE SYNTHESIS AND PROCESSING OF ADVANCED MATERIALS

OVERVIEW

The DOE Center of Excellence for the Synthesis and Processing of Advanced Materials is a distributed center for promoting coordinated, cooperative research partnerships related to the synthesis and processing of advanced materials. It was established by DOE's Division of Materials Sciences, Office of Basic Energy Sciences and the DOE Laboratories in recognition of the enabling role of materials synthesis and processing to numerous materials fabrication- and manufacturing-intensive technologies. The participants include investigators from 12 DOE national laboratories, universities and the private sector. The Center has a technological perspective which is guided a Technology Steering Group.

The current emphasis of the Center is on eight focused multilaboratory projects which draw on the complementary strengths of the member institutions in their ongoing research programs. These seven projects were selected on the basis of the following criteria: (1) scientific excellence, (2) clear relationship to energy technologies, (3) involvement of several laboratories, (4) existing or potential partnerships with DOE Technologies-funded programs, and (5) existing or potential "in-kind" partnerships with private industry.

The eight projects are: (1) Metal Forming, (2) Materials Joining (3) Tailored Microstructures in Hard Magnets, (4) Microstructural Engineering with Polymers, (5) Processing for Surface Hardness, (6) Mechanically Reliable Surface Oxides for High Temperature Corrosion Resistance, (7) High Efficiency Photovoltaics, and (8) Design and Synthesis of Ultrahigh-Temperature Intermetallics. The member laboratories of the Center are: Ames Laboratory (Ames), Argonne National Laboratory (ANL), Brookhaven National Laboratory (BNL), Idaho National Engineering and Environmental Laboratory (INEEL), University of Illinois Frederick Seitz Materials Research Laboratory (UI/MRL), Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), National Renewable Energy Laboratory (NREL), Oak Ridge National Laboratory (ORNL), Pacific Northwest National Laboratory (PNNL), and Sandia National Laboratories (SNL). The Center also includes appropriate university grant research.

Objective

The overall objective of the Center is,

> *To enhance the science and engineering of materials synthesis and processing in order to meet the programmatic needs of the Department of Energy and to facilitate the technological exploitation of materials.*

Synthesis and Processing (S&P) are those essential elements of materials science and engineering (MS&E) that deal with (1) the assembly of atoms or molecules to form materials, (2) the manipulation and control of the structure at all levels from the atomic to the macroscopic scale, and (3) 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 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 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, cost-effective products.

The Center's emphasis is on the elucidation and application of fundamental S&P principles directed toward the rapid improvement or development and ultimate utilization of advanced materials. In order to meet its overall objective, the Center has the following specific objectives:

1) Develop synthesis and processing methodologies to control structure, and thereby materials properties, from the atomic to the macroscopic scale.

2) Discover and develop high-payoff, advanced materials.

3) Integrate fundamental scientific principles with the concurrent development of synthesis and processing in collaboration with DOE technologies-funded programs and with industry.

The Center's Technology Steering Group

A Technology Steering Group (TSG) for the Center has been established. The role of TSG is to become familiar with the Center's technical activities and comment on their technological value, provide information from a technology perspective, help identify technological barriers, influence the direction of the Center's programs, and help develop ideas which can make the Center more effective.

Current TSG membership is as follows:

Member	Affiliation
Dr. Thomas C. Clarke	IBM-Almaden
Dr. Howard Feibus	DOE/Fossil Energy
Dr. David W. Johnson, Jr.	Bell Labs Lucent Technologies
Dr. Hylan B. Lyon	Marlow Industries
Dr. Neil E. Paton	Howmet Corporation
Dr. Charles Sorrell	DOE/Energy Efficiency and Renewable Energy
Dr. John Stringer	Electric Power Research Institute (EPRI)

Materials and Processes Focus of the Center

The current emphasis of the Center is on the eight focused multilaboratory projects cited above.
Each of the projects is coordinated by an appropriate representative from one of the participating institutions. The overall Center coordinator is:
George A. Samara: (SNL/NM)
Phone: (505) 844-6653
Fax: (505) 844-4045
email: gasamar@sandia.gov

A brief description of each project follows:

Metal Forming

Participating Labs: Ames, LBNL, LLNL, LANL, ORNL, PNNL, SNL/CA, SNL/NM
Coordinator: M. Kassner (Oregon State University)
Phone: (541) 737-7023
Fax: (541) 737-2600
email: Kassner@engr.orst.edu
(Included activities: 7, 88, 160, 172, 226, 239)

This project is motivated by the goal of improving fuel efficiency in transportation systems. Achieving this goal requires the use of light weight structural materials which in turn necessitates consideration of aluminum alloys. Unfortunately, compared to steels, Al alloys are more expensive .

The first objective of this project is a scientific understanding of phenomena relating to the forming of aluminum alloys for commercial (especially automotive) applications. This particularly includes recrystallization, which is both poorly understood fundamentally, and poorly predicted during industrial processing. Recrystallization is basically a process by which the material softens by forming new, relatively defect-free, crystallites. The study of recrystallization phenomena includes understanding the precursor states or microstructures.

The second objective is developing equations that will predict, over a complicated thermal and mechanical process, such as will be experienced during industrial processing, the mechanical behavior of aluminum alloys for automotive applications. The equations will consider recrystallization, texture, hardening and dynamic recovery (a less dramatic softening process than recrystallization). No set of constitutive equations has yet effectively modeled these phenomena. The scientific underpinning of the first objective could allow more realistic and versatile constitute equations.

Materials Joining

Participating Labs: Ames, INNEL, LBNL, LLNL, ORNL, PNNL, SNL/CA, SNL/NM
Coordinator: R. B. Thompson (Ames)
Phone: (515) 294-9649
Fax: (515) 294-4456
email: thompsonrb@ameslab.gov
(Included activities: 6, 7, 11, 73, 99, 151, 159, 227, 239, 241)

Materials Joining is an enabling technology in virtually all industrial sectors, and often the reliability of joints is the factor that limits performance. Welding is an old technology, but weld failures are common and some technologically important materials such as aluminum alloys are difficult to weld. Advanced high temperature ceramics and ceramic composites have tremendous potential in energy and related technologies, but there are no reliable methods of joining them. These realities provide the motivation for this project.

The project consists of two tasks. The first entitled "*The Effects of Gradients on Weld Reliability and Performance,*" uses advances in experimental, analytical and computational tools to develop an integrated and quantitative understanding of the origin, extent and effects of gradients in composition, stress, microstructure and properties which occur during various welding processes. Strategies will also be developed to control these gradients which are often the cause of failure. Initial emphasis is on Al-Cu alloys and on Fe-Ni-Cr alloys.

The second task, "*Ceramics and Dissimilar Materials Joining,*" focuses on critical issues in the non-welding joining area which include property mismatch between members to be joined; use temperature limitation; joining temperature limitation; poor wetting, adhesion and/or chemical bonding; potential for use in the field; and manufacturing and/or joint reliability. Some of the initial emphasis is on silicon carbide joining, an area of strong interest to the Fossil Energy program. This part of the work is being done in collaboration with research sponsored by the Continuous Fiber Ceramic Composites Program, Office of Industrial Technologies, Office of Energy Efficiency and Renewable Energy.

Tailored Microstructures in Hard Magnets

Participating Labs: Ames, ANL, BNL, INNEL, LBNL, LLNL, LANL, ORNL
Coordinator: Bob Dunlap (ANL)
Phone: (630) 252-4925
Fax: (630) 252-4798
(Included activities: 1, 68, 73, 127, 146, 171, 198)

Improvements in the properties of permanent (or hard) magnetic materials can lead to lighter, more efficient and longer life motors for energy, transportation and many other industries. A figure of merit for permanent magnet materials is the maximum energy product, W. In some of the best current commercial materials W is ≤50% of its theoretical value. The problem is generally attributed to a lack of understanding of the role of microstructure in determining magnetic properties. Other limitations of current commercial magnetic materials are relatively poor mechanical and corrosion-resistant properties. These properties are also determined largely by microstructure.

The overall objective of this project is to improve hard magnets by understanding, in terms of the microstructures achieved, the magnetic and mechanical properties of materials produced by a number of synthesis and processing (S&P) approaches.

Initial focus is on the technologically important material $Nd_2Fe_{14}B$ as a model system. Specifically, this material is being produced in single crystal, powder, bulk and thin film forms and characterized by state-of-the-art tools. The microstructures developed by the different S&P methods are being compared and modeled. The relationships between microstructure and domain wall pinning, magnetic properties and mechanical properties are being determined. The ultimate goal is to identify S&P approaches which optimize material properties for specific applications.

Microstructural Engineering with Polymers

Participating Labs: Ames, ANL, BNL, INEEL, UI/MRL, LBNL, LLNL, PNNL, SNL/NM
Coordinator: Gregory J. Exarhos (PNNL)
Phone: (509) 375-2440
Fax: (509) 375-2186
email: gj_exarhos@pnl.gov
(Included activities: 2, 225, 241)

This multidisciplinary project is focused on the preparation and properties of advanced polymer and polymer-derived ceramic materials. The research is driven by concepts derived from BES/DMS supported programs. Ongoing work addresses mass transport and diffusion processes not only in blends or composites but in materials which harbor homogeneous micro- or nano-structured domains formed by means of molecular templating routes. Design and processing of polymer-derived materials which are molecularly mixed and which exhibit targeted transport properties will have significant implications for Department of Energy applied technologies. The program provides a fundamental underpinning for the development of new materials to support the electric power, chemical separations, thermal insulation, automotive, building, and membrane, sensor, and catalysis industries. All activities in this project are partitioned among three key topics: (I) molecule directed architectures; (ii) engineered transport materials; (iii) characterization/modeling. .

The resident molecular bonding and network connectivity influence the transport of electrons, ions, molecules, and thermal, and electromagnetic energy through these materials. Based upon modeling studies, preparative routes are developed with which the targeted connectivity can be realized. This research program integrates fundamental materials modeling work with synthesis, chemical and structural characterization, and properties measurements. The goals of this work is to develop next generation polymer-based materials with enhanced transport properties and improved mechanical, thermal, and chemical stability. This engineered multifunctionality requirement presents a materials processing challenge which this multilaboratory effort is poised to address.

Processing for Surface Hardness

Participating Labs: ANL, BNL, LBNL, LLNL, LANL, ORNL, SNL/CA, SNL/NM
Coordinator: J. B. Roberto (ORNL)
Phone: (423) 574-0227
Fax: (423) 574-4143
email: robertojb@ornl.gov
(Included activities: 129, 160, 235, 245)

There exists a broad range of applications for which the ability to produce an adherent, hard, thin, wear-resistant coating plays a vital role. These applications include engine and machine components, orthopedic devices, textile manufacturing components, hard disk media, micromachined sensors and actuators, optical coatings, and cutting and machining tools (e.g., punches, taps, scoring dies, and extrusion dies). Emphasis is placed on development and improvement of processes which are environmentally benign and which provide flexible control over the surface structure and chemistry.

Plasma-based processing is an important component of processes used for the applications listed above. The ability to provide flux, energy, and temporal control of a variety of ions, which is characteristic of plasma-based processing, provides the means to tailor surface hardness and other tribological properties.

The goal of the project is to address critical issues which limit the use of plasma-based processing for surface hardness. Initial emphasis is on plasma ion immersion processing (PIIP), a relatively inexpensive non-line-of-sight-implantation process capable of treating complex-shaped targets without complex fixturing, and on boron-based superhard coatings where the focus is on cubic boron nitride and boron suboxides.

Mechanically Reliable Surface Oxides for High-Temperature Corrosion Resistance

Participating Labs: ANL, INNEL, LBNL, LLNL, ORNL
Coordinator: Linda L. Horton (ORNL)
Phone: (423) 574-5081
Fax: (423) 574-7659
email: hortonLL@ornl.gov
(Included activities: 34, 74, 159, 198)

Protection from corrosion and environmental effects arising from deleterious reactions with gases and condensed products is required to fully exploit the potential of advanced high-temperature materials designed to improve energy efficiency and minimize deleterious environmental impact. The resistance to such reactions is best afforded by the formation of stable surface oxides that are slow growing, sound, and adherent to the substrate and/or by the deposition of coatings that contain or develop oxides with similar characteristics. However, the ability of brittle ceramic films and coatings to protect the material on which they are formed or deposited has long been problematical, particularly for applications involving numerous or severe high temperature thermal cycles or very aggressive environments. This lack of mechanical reliability severely limits the performance or durability of alloys and ceramics in many high-temperature industrial applications and places severe restrictions on deployment of such materials. The beneficial effects of certain alloying additions on the growth and adherence of protective oxide scales on metallic substrates are well known, but satisfactory broad understandings of the mechanisms by which scale properties and coating integrity (that is, corrosion resistance) are improved by compositional, microstructural, and processing modifications are lacking.

The objective of this task is to systematically generate the knowledge required to establish a scientific basis for the design and synthesis of improved (slow growing, adherent, sound) protective oxide coatings and scales on high temperature materials without compromising the requisite bulk material properties. Specific objectives are to: (1) systematically investigate the relationships among substrate composition and properties and scale/coating failure using a mix of relevant microstructural and mechanical characterization techniques and modeling, and (2) identify conditions leading to more damage-tolerant coatings and scales that are amenable to legitimate synthesis routes. The initial emphasis is on alumina scales and coatings. The work is co-sponsored by the Office of Advanced Research, Fossil Energy Program, and the Electric Power Research Institute (EPRI).

High Efficiency Photovoltaics

Participating Labs: Ames, ANL, BNL, INNEL, UI/MRL, LBNL, LLNL, NREL, ORNL, PNNL, SNL/CA, SNL/NM, Caltech, MIT, SUNY, U.Florida, UCSB, U.Utah, Washington State U.
Coordinator: S. K. Deb/J. Benner (NREL)
Phone: (303) 384-6405 / (303) 384-6496
Fax: (303) 384-6481
email: satyen_deb@nrel.gov
(Included activities: 31, 129, 146, 182, 233)

Advances in the technology of solar photovoltaic (PV) energy conversion are critically dependent on the fundamental understanding of the synthesis and properties of the materials that compose solar cells. Reduced cost, improved conversion efficiency, and long-term stability are the major objectives of the DOE Photovoltaics Program. Thin-film semiconductor materials and device technologies are key to achieving these objectives. Currently, there are several important classes of thin-film PV materials at various stages of research and development, but in all cases there is a lack of understanding of the fundamental scientific issues associated with each of these technologies. Therefore, this program is motivated by the scientific exploration of new solid-state physics as it relates to photon absorption and carrier transport, novel materials synthesis techniques, the characterization and control of defect structures, and ultimately designs of new material architectures.

The project is focused on two areas: (1) Silicon-Based Thin Films, in which key scientific and technological problems involving amorphous and polycrystalline silicon thin films will be addressed; and (2) the Next Generation Thin Film Photovoltaics, which will be concerned with the possibilities of new advances and breakthroughs in the materials and physics of photovoltaics using non-silicon-based materials.

Design and Synthesis of Ultrahigh-Temperature Intermetallics

Participating Labs: Ames, ANL, INEEL, UI/MRL, LBNL, LLNL, LANL, ORNL, SNL/CA

Coordinators: Roddie R. Judkins (ORNL) and R. Bruce Thompson (Ames)
Phone: (423) 574-4572 / Phone: (515) 294-9649
Fax: (423) 574-5812 / Fax: (515) 294-4456
Email: judkinsrr@ornl.gov / Email: thompsonrb@ameslab.gov
(Included activities: 158)

High-temperature structural materials are critically needed for improving the thermal efficiency and reliability of energy conversion systems and advanced engine systems. The currently available alloys, such as Ni-base single-crystal superalloys, are limited to use temperatures of about 1100°C. Aluminide alloys based on NiAl, which are currently under development, have the potential to be used up to 1200°C. However, many applications require temperature capabilities that exceed this temperature by at least 200°C. The melting temperature (T_m) of a material for structural applications at 1400°C should be greater than 2000°C so that, at most, 0.75 T_m is research during service, and appreciable high-temperature strength is maintained. Of the potential candidate systems, transition-metal silicides are particularly attractive owing to their high melting points, good creep properties, and promising oxidation resistance.

The board objective of this Project is to generate the knowledge required to establish a scientific basis for the processing and design of transition-metal silicides with improved metallurgical and mechanical properties at ambient and high temperatures. Its ultimate goals is to develop scientific principles to design new-generation materials based on silicides for structural applications at temperature at and above 1400°C.

The Projects consists of three major tasks: First-Principles Calculations, Atomistic Simulations and Mechanistic Modeling; Experimental Study of Structure and Properties; and Innovative Materials Processing and Fabrication. Emphasis in on Mo_5Si_3-base alloys as guided by input from DOE's Fossil Energy (FE) Advanced Research and Technology Development (AR&TD) Materials Program and Energy Efficiency and Renewable Energy (EERE) Advanced Industrial Materials (AIM) Program.

SECTION E

Major User Facilities

(Large Capital Investment)

ADVANCED PHOTON SOURCE

Argonne National Laboratory
Argonne, Illinois 60439

The Advanced Photon Source (APS) is a powerful synchrotron radiation research facility. It is the nation's most brilliant source of X-ray beams in the energy range from 3 to 300KeV. The APS design is optimized to employ special magnetic arrays called "insertion devices" which generate monoenergetic; tunable proton beams. X-ray beam brilliances of the order of 10^{18} photons/second mm^2 mr^2 (0.1% Bandwidth) at 10 KeV are produced. These brilliant X-ray beam probe material structure in greater detail than ever before, opening new vistas of research in materials sciences, chemistry, physics, biology, energy sciences and applied technologies. The facility provides up to 70 independent X-ray beamlines for research by teams of researchers from universities, industry, national laboratories, and other research institutions.

User Mode

APS is available at no charge to qualified scientists engaged in fundamental, non-proprietary research. Proprietary research can be carried out at a full cost recovery basis. Independent investigators may access the facility by submitting a technically-competitive proposal to any research team operating beamlines at the APS. Collaborative Access Teams (CATs) are granted continuing access to the APS facilities upon satisfactory peer review by an independent Program Evaluation Board. Full details of the APS User program, including a APS User Guide, can be obtained from the APS User Office, Building 401, Argonne National Laboratory or by browsing the APS world wide web site (http://www.aps.anl.gov).

Persons to Contact for Information

D. E. Moncton, Associate Laboratory Director
Argonne National Laboratory
APS Building 401
9700 South Cass Avenue
Argonne, IL 60439

(630) 252-7950
Fax: (630) 252-4599
E-mail: dem@aps.anl.gov

User Office

(630) 252-5981
Fax: (630) 252-9250
E-mail: apsuser@aps.anl.gov

DESCRIPTIONS OF ADVANCED PHOTON SOURCE COLLABORATIVE ACCESS TEAMS

SRI-CAT,Sectors1-3 The primary focus of the Synchrotron Radiation Instrumentation-CAT or SRI-CAT is to develop critical beamline instrumentation that can be used by the entire APS community and to conceive and implement experimental techniques that exploit the unique properties of APS radiation. This CAT contains both instrument development scientists from the APS and other national laboratories and scientific members from national laboratories, academia, and industry. Dennis Mills (Experimental Facilities Division/APS) is the Director of SRI-CAT (telephone: 630/252-5680; email: dmm@aps.anl.gov).

DND-CAT,Sector 5 DND-CAT is the DuPont-Northwestern-Dow Collaborative Access Team. Although many fields of materials science and engineering are represented in the planned research program, the scientific thrust is concentrated in three main areas: (1) crystallography; (2) the study of two dimensional or quasi-two dimensional atomic structures (surfaces, interfaces and thin films); and (3) polymer science and technology. The DND-CAT Director is Joe Georgopoulos (DND-CAT) Synchrotron Research Center; telephone: 630/252-0221; email: joe_g@nwu.edu).

μ-CAT,Sector 6 The Midwest Universities-CAT (μ-CAT) beamlines are designed for studies in materials science, with surface diffraction, diffraction from small samples, and control of polarization for studies of magnetic systems as areas of key interest. Institutional affiliations of μ-CAT members include Georgia Tech., Ames Laboratory/Iowa State University, Kent State, SUNY at Stony Brook, University of Missouri at Columbia, University of Nebraska at Lincoln, University of Wisconsin at Madison, and Washington University. The Director of μ-CAT is Alan Goldman (Iowa State University; telephone: 515/294-3585; e-mail: goldman@ameslab.gov).

MHATT-CAT,Sector 7 The Center for Real-Time X-ray Studies-CAT (MHATT-CAT) has three institutional members: University of Michigan, Howard University, and Bell Laboratories. This sector will consist of two 60-meter-long beamlines instrumented for time-resolved experiments in X-ray scattering and spectroscopy. The primary scientific thrust of MHATT-CAT will be to study the different dynamical processes that occur in complex materials, ranging from internal conformational changes in proteins to relaxation phenomena in glasses. MHATT-CAT's Director is Walter Lowe (Howard University; telephone: 301/419-9030; e-mail: lowe@mhattcat.howard.edu).

IMM-CAT,Sector 8 The scientific program of the IBM-MIT-McGill-CAT (IMM-CAT) focuses on dynamic phenomena in materials science and condensed matter physics. The insertion-device beamline will be optimized for scattering experiments, and the bending-magnet beamline will be optimized for resonant scattering and spectroscopy. The Director of IMM-CAT is Simon Mochrie (MIT; telephone: 617/253-6588; e-mail: simon@lindy.mit.edu).

CMC-CAT, Sector 9 The Complex Materials Consortium-CAT (CMC-CAT) is developing a beamline optimized for several experimental techniques used to study complex materials (polymers, surfactants, liquid crystals, biomaterials, membranes, and thin molecular films of hydrocarbons on solid or liquid surfaces, etc.). Institutional affiliations of key CAT members include: Argonne National Laboratory, Brookhaven National Laboratory, Exxon Research and Engineering, Los Alamos National Laboratory, Princeton University, University of California-Santa Barbara, University of Pennsylvania, and University of Tennessee/Oak Ridge National Laboratory. The CMC-CAT Director is Doon Gibbs (Brookhaven National Laboratory; telephone: 516/344-4608; e-mail: doon@solids.phy.bnl.gov).

MR-CAT, Sector 10 The Materials Research-CAT (MR-CAT) includes scientists from Amoco, Argonne National Laboratory's Chemical Technology/Geosciences Division, the Illinois Institute of Technology, Northwestern University, the University of Notre Dame, and the University of Florida. The scientific studies planned by the CAT include time-resolved scattering and spectroscopy, spatially resolved measurements, and *in situ* measurements. These techniques will be used to study a variety of systems ranging from semiconductor interfaces to catalysts to "soft" condensed matter systems. The MR-CAT Director is Bruce Bunker (Notre Dame; telephone: 219/631-7219; e-mail: bruce.bunker.1@nd.edu).

BESSRC-CAT, Sectors 11 and 12 The Basic Energy Sciences Synchrotron Radiation Center-CAT (BESSRC-CAT) consists of scientists from the Chemistry, Materials Science and Physics Divisions of ANL, as well as from the Geosciences groups at ANL and Northern Illinois University. The primary scientific focus is on materials, chemical, and geological sciences; and atomic physics. BESSRC-CAT's two sectors will contain four beamlines and 10 distinct instrumented stations, seven of which will be equipped initially. Two types of insertion devices will be used for the insertion-device beamlines: an undulator A and an elliptical multipole wiggler. The BESSRC-CAT Director is Pedro A. Montano (ANL, Materials Science Division; telephone: 630/252-6239; e-mail: Pedro_Montano@qmgate.anl.gov).

CARS-CAT, Sectors 13-15 The Consortium for Advanced Radiation Sources-CAT (CARS-CAT) is a multi-disciplinary, multi-institution, multi-sector CAT. It includes The University of Chicago, Northern Illinois University, and Southern Illinois University as primary institutional members and serves four national user groups (BioCARS, ChemMatCARS, GeoCARS, and SoilEnviroCARS). The University of Chicago serves as the managing agent for this CAT. The scientific program and experiments planned for CARS beamlines are designed to exploit the unique features of X-rays emitted by both undulator and wiggler sources through X-ray scattering, spectroscopy, and microprobe approaches. Both spatially resolved and time-resolved experiments are planned. The CARS-CAT Director is Keith Moffat (The University of Chicago; telephone: 312/702-9950; e-mail: moffat@cars1.uchicago.edu).

IMCA-CAT, Sector 17 The Industrial Macromolecular Crystallography Association-CAT (IMCA-CAT) is a consortium of crystallographic groups from 12 companies with major pharmaceutical research laboratories in the United States. This group was organized to build and operate two beamlines at the APS dedicated to protein crystallography, with the goal of providing data for structure-based drug design. Both proprietary and non-proprietary research will be conducted on IMCA-CAT beamlines. The Director of IMCA-CAT is Andrew Howard (Illinois Institute of Technology; telephone: 312/567-5881; e-mail: ahoward@sparky.csrri.itt.edu).

BIO-CAT, Sector 18 The Biophysics-CAT (Bio-CAT) plans to study the structure and dynamics of biological and related systems at the molecular level, with a focus on partially ordered samples such as membranes, fibers, and solutions. The primary research techniques will be resonant (anomalous) and nonresonant X-ray diffraction, and X-ray absorption fine structure (XAFS) spectroscopy. The Director of Bio-CAT is Grant Bunker (Illinois Institute of Technology; telephone: 312/567-3385; e-mail: bunker@biocat1.iit.edu).

SBC-CAT, Sector 19 The Structural Biology Center-CAT (SBC-CAT) is building a national user facility at the APS for studies in macromolecular crystallography. The SBC will provide crystallographers with access (through peer-reviewed proposals) to both an insertion-device and a bending-magnet beamline optimized for studies in macromolecular crystallography, plus a full complement of instrumentation, ancillary facilities, software, and support staff. The SBC-CAT Director is Edwin Westbrook (Argonne National Laboratory, Center for Mechanistic Biology; telephone: 630/252-3983; e-mail: westbrook@anl.gov).

PNC-CAT, Sector 20 The Pacific Northwest Consortium-CAT (PNC-CAT) is building beamlines with innovative instruments, including a scanning X-ray microprobe with 0.1-µm resolution and instrumentation for material analysis emphasizing energy scanning (either in the incident or scattered X-rays) techniques such as XAFS, DAFS, inelastic X-ray resonance and Raman scattering. Research is planned in a variety of areas, with an emphasis on environmentally related problems. The optics include a toroidal mirror, a capillary concentrator, and a Kirkpatrick-Baez mirror pair. Instrumentation includes an energy analyzer for scattered x-rays, an MBE facility with a UHV chamber, and imaging capabilities. Primary institutional members of this CAT include the University of Washington, Pacific Northwest National Laboratories, and Simon Fraser University. The Director of PNC-CAT is Edward Stern (University of Washington; telephone: 206/543-2023; e-mail: stern@phys.washington.edu).

UNI-CAT, Sector 33 The University-National Laboratory-Industry CAT (UNI-CAT) consists of four primary institutional members: University of Illinois at Urbana-Champaign, Oak Ridge National Laboratory, National Institute of Standards and Technology, and UOP Research and Development. The focus of this CAT is the development of state-of-the-art instrumentation to allow structural characterization at the atomic level. Special capabilities include focusing beam optics, an ultrahigh-vacuum molecular beam epitaxy (MBE) chamber, a chemical-vapor deposition (CVD) facility, topography, microscopy, and ultrasmall-angle X-ray scattering (USAXS) apparatus, instrumentation for time-resolution scattering experiments, and reactive environment X-ray absorption spectrometry (XAS) capabilities. The Director of UNI-CAT is Haydn Chen (University of Illinois; telephone: 217/244-4666; e-mail: chen@uimrl7.mrl.uiuc.edu).

MICRO-CAT, Sector 34 A Micro-Investigation of Composition Research Organization CAT (MICRO-CAT) proposes to develop and operate a microprobe facility with wide-ranging applications in the fields of materials science, chemistry, geochemistry, environmental science, and medicine. Materials science studies will include the measurement of impurity effects and strains in crack growth and fracture; ductility of grain boundaries; the study of creep, ceramics, and reinforced composites; diffusion studies; the study of integrated circuits and microchips; and radiation effects. Environmental and biological studies include such things as measurement of trace element distribution in tree rings, fish scales, clam shells, and other time-dependent growth tissues where contamination levels can be related to chronology of exposure, and the measurement of contamination transport by small particles. The director of MICRO-CAT is Gene E. Ice (Oak Ridge Natl. Lab.; telephone 423/574-2744; fax (423)574-7659.

INTENSE PULSED NEUTRON SOURCE

Argonne National Laboratory
Argonne, Illinois 60439

IPNS is a pulsed spallation source dedicated to research on condensed matter. The source has some unique characteristics that have opened up new scientific opportunities:

- high fluxes of epithermal neutrons (0.1-10 eV)
- solid methane moderation procuding high fluxes of cold neutrons (λ>4Å)
- pulsed nature, suitable for real-time studies and measurements under extreme environments
- 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 magnetic moments) in a material and the relation of this arrangement to its physical and chemical properties, and inelastic neutron scattering, concerned with processes where the neutron exchanges energy and momentum with the system under study and thus probes the dynamics of the system at a microscopic level. At the same time, the facilities are used for technological applications, such as stress distribution in materials and characterization of zeolites, ceramics, polymers, and hydrocarbons.

USER MODE

IPNS is available without charge to qualified scientists doing fundamental research. Selection of experiments is made on the basis of scientific merit by a Program Committee consisting of eminent scientists, mostly from outside Argonne. Scientific proposals (4 pages long) are submitted twice a year and judged by the Program Committee. Full details, including a User's Handbook, Proposal and Experimental Report Forms, can be obtained from the Scientific Secretary, IPNS, Building 360, Argonne National Laboratory or at htt://www.pns.anl.gov. 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 IPNS Building 360 9700 South Cass Avenue Argonne, IL 60439	(630) 252-4999 FAX (630) 252-4163 E-mail: brown@anlpns.anl.gov
Scientific Secretary	(630) 252-6600

IPNS EXPERIMENTAL FACILITIES

Instrument (Instrument Scientist)	**Range** Wave-vector* ($Å^{-1}$)	Energy (eV)	**Resolution** Wave-vector ($Å^{-1}$)	Energy (eV)
Special Environment Powder Diffractometer (J. D. Jorgensen/S. Short)	0.5-50	**	0.35%	**
General Purpose Powder Diffractometer (J. Richardson/R. Thomas)	0.5-100	**	0.25%	**
Single Crystal Diffractometer (A. J. Schultz/R. Vitt)	2-20	**	2%	**
Low-Res. Medium-Energy Chopper Spectrometer (R. Osborn/R. Zugler)	0.1-30	0-0.6	0.02 k_o	0.05 E_o
High-Res. Medium-Energy Chopper Spectrometer (C.-K. Loong/O. Yocum)	0.3-9	0-0.4	0.01 k_o	0.02 E_o
Small Angle Diffractometer (P. Thiyagarajan/D. Wozniak)	0.006-0.35	**	0.004	**
Small Angle Neutron Diffractometer (SAND) (P. Thiyagarajan/D. Wozniak)	0.006-2.0	**	0.004	**
Polarized Neutron Reflect. (POSY) (G. P. Felcher/R. Goyette)	0.0-0.07	**	0.0003	**
Neutron Reflect. (POSY II) (A. Wong/R. Goyette)	0.0-0.25	**	0.001	**
Quasi-Elastic Neutron Spectrometer (F. Trouw/C. Johnson)	0.42-2.59	0-0.1	~0.2	70 $\mu eV^{<->}$ 0.01ΔE
Glass, Liquid and Amorphous Materials Diffractometer*** (D. L. Price/K. Volin)	0.05-25 0.1-45	** **	~0.5% cotθ ~1.0% cotθ	** **
High Intensity Powder Diffractometer (A. J. Schultz/R. Vitt)	0.5-25 1.8-50	** **	1.8-3.5% 0.9%	** **

* Wave-vector, $k = 4\pi \sin\theta/\lambda$.
** No energy analysis.
*** Two sample positions
<-> Elastic and inelastic resolution

Not Yet in the User Program
Chemical Excitation Spectrometer (CHEX)

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 = 0.5×10^{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 ($\gamma > 4$ Å). A polarized beam spectrometer, triple-axis spectrometers and small-angle scattering and neutron reflectometry 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.

PERSON TO CONTACT FOR INFORMATION

Rae Greenberg
Brookhaven National Laboratory
Building 510A
P. O. Box 5000
Upton, NY 11973-5000

(516) 344-5564
Fax (516) 344-5888
email: greenbel@bnl.gov
www: http://neutron.chm.bnl.gov/HFBR/index.html

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 diffraction; polarized beam. Energy range: 2.5 MeV, < E_o < 200 MeV Q range: 0.03 < Q < 10$Å^{-1}$
Small Angle Neutron Scattering (H9B)	Studies of large molecules. Located on cold source with 50 x 50 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
Neutron Spectrometer (H5)	Inelastic scattering Diffuse scattering Powder diffraction; 15 ^{3}He detectors covering 90°
(n, γ) Spectrometer (H1B)	Neutron capture studies Energy range: 0.025 eV <E_o<25 KeV
Neutron Reflectometer (H9D)	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, $\Delta d/d = 5 \times 10^{-4}$Ge(511) vertical focussing monochromator. 64 He^3 detectors, covering 160°
Irradiation Facilities 7 Vertical Thimbles	Neutron activation; production of isotopes; thermal flux: 8.3 x 10^{14} neutrons/cm^2-sec; fast (> 100 MeV) flux: 3 x 10^{14} neutrons/cm^2-sec.

NATIONAL SYNCHROTRON LIGHT SOURCE

Brookhaven National Laboratory
Building 725B, P.O. Box 5000
Upton, New York 11973-5000

The National Synchrotron Light Source (NSLS) is the largest facility in the U.S. dedicated to the production of synchrotron radiation. Funded by the Department of Energy as a user facility, construction on the NSLS began in 1977 with VUV Ring operation commencing in 1982 and X-Ray Ring operation in 1984. Since then, the facility has undergone a major 4-year upgrade and is continually improved to take advantage of the latest technology in storage rings, beamline optics, and insertion devices.

The NSLS operates two electron storage rings producing high brightness synchrotron radiation in the infrared, visible, ultraviolet, and X-ray regions of the electromagnetic spectrum. Insertion devices installed in the straight sections of the rings provide radiation that is anywhere from one to several orders of magnitude brighter than the radiation from bending magnets. The VUV Ring operates at 800 MeV with a critical energy of 486 eV. It has 17 beam ports split into 32 experimental stations, or beamlines, and also supports two insertion devices. The X-Ray Ring operates at 2.5 GeV, 300 mA, with a critical energy of about 5 keV. It has a total of 30 beam ports split into 61 beamlines and currently supports 5 insertion devices: two undulators, a superconducting wiggler, and two hybrid wigglers. There are also a number of beamlines devoted to machine diagnostics and R&D. The NSLS facility has user laboratories and a wide range of research equipment for basic and applied studies in condensed matter, surface science, photochemistry and photophysics, lithography, crystallography, small-angle scattering, metallurgy, X-ray microscopy, topography, etc. Detailed information about beamline research programs, experimental apparatus, and optical configurations is available from the NSLS User Administration Office and the NSLS Home Page.

USER MODES

Over 2,200 scientists from approximately 370 institutions came to the NSLS during 1997. The NSLS is a national user facility available without charge to university, industrial, national laboratory, and government users. In addition, a program is available to assist faculty/student research groups who have limited grant support and wish to defray travel expenses to the NSLS. Proprietary work can be done on a full cost recovery basis with the option to retain title to inventions resulting from research at the NSLS.

There are several ways of using NSLS experimental facilities. A large fraction of the beamlines have been designed and constructed by Participating Research Teams (PRTs). PRTs are comprised of one or more research teams from industry, universities, and other laboratories with large, long-range programs which have been approved by the NSLS Scientific Advisory Committee (SAC). The PRT members are given priority for up to 75 percent of their beamline's operational time, and their programs are reviewed by the SAC every 3-years. Peer-reviewed General User proposals are scheduled on both PRT beamlines and on beamlines built by the NSLS for the general community. The NSLS facility operates throughout the year with beam time scheduled in 4-month cycles. Deadlines for General User proposals are September 30, January 31, and May 31. Information about submitting research proposals, becoming a PRT, or applying for financial assistance may be obtained from the NSLS User Administration Office or the world wide web at www.nsls.bnl.gov.

PERSON TO CONTACT FOR INFORMATION

Eva Z. Rothman, User Administrator
NSLS Bldg. 725B
Brookhaven National Laboratory
P.O. Box 5000
Upton, NY 11973-5000

(516) 344-7114
Fax (516) 344-7206

E-mail: ezr@bnl.gov
NSLS Home Page: http://www.nsls.bnl.gov

NATIONAL SYNCHROTRON LIGHT SOURCE (continued)

NSLS TECHNICAL DATA

STORAGE RINGS	KEY FEATURES
VUV electron	17 ports; Ec - 25.3 angstroms; 0.808 GeV electron energy
X-ray electron	30 ports; Ec - 2.48 angstroms; 2.584 GeV electron energy

RESEARCH AREA	WAVELENGTH RANGE (Angstroms)	ENERGY RANGE (eV)	NUMBER OF BEAMLINES
Absorption Spectroscopy	0.35 - 2480	5 - 35,000	24
Circular Dichroism	10.3 - 5904	2.1 - 1200	2
High Pressure Physics	1 - 10,000 m	0.124 - 1240 meV	2
	WB; 0.12 - 1.24	WB; 10,000 - 100,000	2
High Q-Resolution Scattering	WB; 0.12 - 6.20	WB; 2000 - 100,000	15
Imaging:			
Medical	WB; 0.12 - 1.24	WB; 10,000 - 100,000	2
Tomography	WB; 0.12 - 3.10	WB; 4000 - 100,000	3
X-ray Microprobe	WB; 0.12 - 3.10	WB; 4000 - 100,000	3
X-ray Microscopy/Holography	10 - 80	155 - 1240	1
X-ray Topography	WB; 0.41 - 3.10	WB; 4,000 - 30,000	2
Infrared Spectroscopy	1 - 10,000 m	0.124 - 1240 meV	2
Lithography	124 - 4133	3 - 100	1
Nuclear Physics	---	80 - 400 (meV)	1
Photoemission Spectroscopy	2.10 - 6200	2 - 5900	19
Photoionization	2.10 - 4133	3 - 5900	3
Protein Crystallography	WB; 0.41 - 3.10	WB; 4,000 - 30,000	6
Radiometry	WB; 8.27 - 248	WB; 50 - 1500	1
Small Angle Scattering:			
Biology	0.66 - 5.90	2100 - 18,800	2
Materials Science	0.36 - 6.20	2000 - 34,000	4
Small Molecule Crystallography:			
Powder	WB; 0.12 - 3.10	WB; 4000 - 100,000	4
Single Crystal	0.21 - 6.20	2000 - 59,400	7
Standing Waves	WB; 0.62 - 6.89	WB; 1800 - 20,000	2
Surface Scattering/X-ray Reflectivity	WB; 0.48 - 6.20	WB; 2000 - 26,000	10
Time Resolved Fluorescence	1393 - 5904	2.1 - 8.9	1
UV Reflectometry	WB; 8.27 - 6200	WB; 2 - 1500	2
X-ray Emission Spectroscopy	2.48 - 50	248 - 5000	2

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

MANUEL LUJAN JR. NEUTRON SCATTERING CENTER

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

The Manuel Lujan Jr. Neutron Scattering Center (Lujan Center) 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 Neutron Science Center (LANSCE) 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, the Lujan Center has the world's highest, peak thermal flux for neutron scattering research. Current research programs at the Lujan Center use the following instruments: a chopper spectrometer (PHAROS) for Brillouin scattering; a filter difference spectrometer (FDS) for vibrational spectroscopy by inelastic neutron scattering; a Laue-TOF single-crystal diffractometer (SCD); a high-intensity powder diffractometer (HIPD) for structural studies of liquids, amorphous materials, and crystalline powders; a neutron powder diffractometer (NPD) with the highest resolution in the U.S.; a low-Q diffractometer (LQD) for small-angle scattering studies; and a surface profile reflectometer (SPEAR) for studies of surface structure.

USER MODE

The Lujan Center provides neutron scattering facilities for several communities. Research programs cover a broad range: solid-state physics, chemistry, metallurgy, crystallography, structural biology, materials science, and nuclear physics. Since FY 1996, the Lujan Center is funded by DOE, Office of Defense Programs for science-based stockpile stewardship (SBSS). Proposed experiments under the SBSS program will be reviewed by a panel of scientists and members of the defense community. Program priority will be evaluated in addition to scientific merit. The Lujan Center also operates a formal user program funded by DOE, Basic Energy Sciences. Scientists from universities, industry, and national laboratories may again apply for beam time by submitting short proposals that will be subjected to appropriate peer review. DOE cost-recovery rules apply to proprietary experiments. The Lujan Center sponsors spectrometer development teams (SDTs) that are guaranteed access to a beamline for a negotiated period in exchange for financial participation in constructing a neutron spectrometer or ancillary equipment.

CONTACT FOR USER INFORMATION

LANSCE User Office		(505) 665-1010
Mail Stop H805	Fax:	(505) 665-8604
Los Alamos National Laboratory	E-Mail:	lansce_users@lanl.gov
Los Alamos, NM 87545	WWW:	http://www.lansce.lanl.gov

MANUAL LUJAN JR. NEUTRON SCATTERING CENTER (continued)

TECHNICAL DATA

Proton Source	LANSCE linac
Proton Source Energy	800 MeV
LANSCE Proton Current	100 μA
Proton Pulse Width	0.27 μs
Repetition Rate	20 Hz
Epithermal Neutron Current (n/eV.Sr.S)	4.5×10^{12}/E
Peak Thermal Flux (n/cm^2.S)	$2A \times 10^{16}$

INSTRUMENTS

32-m Neutron Powder Diffractometer (M. Bourke, Responsible) E-mail: bourke@lanl.gov	Powder Diffraction Wave vector 0.3-25 $Å^{-1}$ Resolution 0.13%
Single Crystal Diffractometer (D. Argyriou) E-mail: argyriou@lanl.gov	Laue time-of-flight diffractometer Wave vectors: 1-15 $Å^{-1}$ Resolution 1% typical
High Intensity Powder Diffractometer (R. VonDreele, Responsible) E-mail: vondreele@lanl.gov	Powder diffraction resolution: 0.5% liquids and amorphous materials diffraction resolution: 3% Wave vectors: 0.1-60 $Å^{-1}$
Low Q Diffractometer (R. Hjelm, Responsible) E-mail: hjelm@lanl.gov	Small angle scattering at a liquid hydrogen cold source Wave vectors: 0.003-0.15 $Å^{-1}$
Reflectometer (G. Smith, Responsible) E-mail: gsmith@lanl.gov	Surface reflection at grazing incidence. Wave vectors: polarized 0.007 to 0.15 $Å^{-1}$; unpolarized 0.008 to 0.3 $Å^{-1}$
Chopper Spectrometer (R. Robinson, Responsible) E-mail: rrobinson@lanl.gov	Inelastic scattering at small scattering angles. Energy trans.: 1-1700 meV Incident energy resolution: 0.5%
Filter Difference Spectrometer (J. Eckert, Responsible) E-mail: juergen@lanl.gov	Inelastic neutron scattering, vibrational spectroscopy Energy trans: 13-620 meV Resolution: 1.5 - 6-5%

NEUTRON SCATTERING AT THE HIGH FLUX ISOTOPE REACTOR

Solid State and Chemistry Divisions
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

The neutron scattering facilities at the High Flux Isotope Reactor (HFIR) are used for long-range basic research on the structure and dynamics of condensed matter. Active programs exist on the magnetic properties of matter, lattice dynamics, defect-phonon interactions, phase transitions, crystal structures, polymers, micelles, ferrofluids, ceramics, and liquid crystals. The HFIR is an 85-MW, light-water moderated reactor. The central flux is 4 x 10^{15} neutrons/cm^2-sec, and the flux at the inner end of the beam tubes is slightly less than 10^{15} n/cm^2-sec. A wide variety of neutron scattering instruments have been constructed with the support of the Division of Materials Sciences. Facilities are available for studies of materials at low and high temperatures, high pressures, and high magnetic fields.

USER MODE

These facilities are open for use by outside scientists on problems of high scientific merit. Written proposals are reviewed for scientific feasibility by an external review committee. It is expected that all accepted experiments will be scheduled within six months of the receipt of the proposal. No charges for the use of the beams will be assessed for research to be published in the open literature. The cost of extensive use of ORNL shop or computer facilities must be born by the user. Inexperienced users will normally collaborate with an ORNL staff member. Proprietary experiments can be carried out after a contract has been arranged based on full cost recovery, including a charge for beam time. A brochure describing the facilities and a booklet giving user procedures is available on request.

PERSON TO CONTACT FOR INFORMATION

G. D. Wignall — (423) 574-5237 — Small Angle Neutron Scattering
Solid State Division
Oak Ridge National Laboratory
Oak Ridge, TN 37831-6393

B.C. Chakoumakos — (423) 574-5235 — Powder and single-crystal structure
Solid State Division
Oak Ridge National Laboratory
Oak Ridge, TN 37831-6393

S. E. Nagler — (423) 574-5420 — Triple-axis spectrometry
Solid State Division
Oak Ridge National Laboratory
Oak Ridge, TN 37831-6393

W. A. Hamilton — (423) 576-6068 — Reflectometry
Solid State Division
Oak Ridge National Laboratory
Oak Ridge, TN 37831-6393

NEUTRON SCATTERING AT THE HIGH FLUX ISOTOPE 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 7 T, Horizontal fields to 5 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}s at sample with 40 min collimation
HB-3A	Double-crystal small-angle diffractometer, Beam size - 4 x 2 cm max, Wavelength = 2.6 angstroms, Flux - 10^4 n/cm^{2}s, Resolution - 4 x 10^{-5} angstroms^{-1}
HB-4A	Wide-angle time-slicing diffractometer, Beam size - 2 x 3.7 cm max, Wavelength = 1.537 angstroms, Flux - 2 x 10^6 n/cm^{2}s with 9 min collimation, Curved linear position sensitive detector covering 130°
HB-4	Correlation chopper, Beam size - 5 x 3.7 cm, Flight path - 1.5 m, 70 detectors covering 130°, Variable E_o, Variable pulse width
	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
HB-3B	Reflectometer, 2.59-Å Horizontal Reflection Plane. 2-mm resolution with linear position-sensitive detector at 3 m from the sample.

STANFORD SYNCHROTRON RADIATION LABORATORY
STANFORD LINEAR ACCELERATOR CENTER

Stanford University
Stanford, California 94309-0210

SSRL is a National Users' Research Laboratory for the application of synchrotron radiation to research, that includes but not limited to, biology, chemistry, engineering, geology, materials science, medicine and physics. In addition to scientific research utilizing synchrotron radiation the Laboratory program includes the development of advanced sources of synchrotron radiation (e.g., insertion devices for the enhancement of synchrotron radiation as well as modifications of SPEAR). SSRL presently has 26 experimental stations with 4 more under construction or commissioning. Three of these are contained in an integrated structural molecular biology facility to be completed in 1997. 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. X-ray and VUV photoemission and photoelectron diffraction studies of electronic states and atomic arrangements in condensed and gaseous matter. Semiconductor and thin film processing and magnetic properties of thin films using circular polarization. SSRL serves over 1,000 scientists from 169 institutions working on 266 active proposals. The Laboratory has rapidly growing programs in applications of synchrotron radiation to the study of biological systems and molecular environmental science. 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.

USER MODE

SSRL is a user-oriented facility which welcomes proposals for experiments from all qualified scientists. SSRL operates for users approximately 9 months per year. Over 85 percent of the beam time is available for the general user. Access is gained through proposal submittal and peer review. An annual Activity Report is available on request. It includes progress reports on about 100 experiments plus descriptions of recent facility developments. The booklets "Proposal Submittal and Scheduling Procedures" and "SSRL Experimental Stations" provide detailed information on proposal submittal and experimental station characteristics.

PERSON TO CONTACT FOR INFORMATION

Artie Bienenstock (415) 926-3153
SSRL FAX: (415) 926-4100
P. O. Box 4349
Stanford, CA 94305

CHARACTERISTICS OF SSRL EXPERIMENTAL STATIONS

SSRL presently has 26 experimental stations on 22 beam ports with 4 more stations under construction/commissioning.

	Horizontal Angular Acceptance (mrad)	Mirror Cut Off (keV)	Monochromator	Energy Range (eV)	Resolution ΔE/E	Approximate Spot Size Hgt x Wdth (mm)	Instrumentation
INSERTION DEVICE STATIONS							
WIGGLER LINES - X-RAY							
End Stations							
4-2 (4 periods)							
Focused	2.0	10.2	Double Crystal	2400–10200	$\sim5 \times 10^{-4}$	0.5 × 4.0	
Unfocused	1.0		Double Crystal	2400–45000	$\sim10^{-4}$	2.0 × 20.0	
4-2 SAXS	0.5–2.0	10.2	Double Crystal	2400–10200	$\sim5 \times 10^{-4}$	0.5 × 4.0	SAXS Camera
	0.5–2.0	10.2	Multilayers	7000–10200	3×10^{-2}	0.5 × 4.0	SAXS Camera
6-2 (27 periods)							
Focused	2.3	22	Double Crystal	2050–21000	$\sim5 \times 10^{-4}$	0.5 × 4.0	
Unfocused	1.0		Double Crystal	2050–32000	$\sim10^{-4}$	2.0 × 20.0	
7-2 (4 periods)							6-circle Diffractometer
Focused	2.0	10.2	Double Crystal	2400–10200	$\sim5 \times 10^{-4}$	1.0 × 4.0	
Unfocused	1.0		Double Crystal	2400–45000	$\sim10^{-4}$	2.0 × 20.0	
9-2 (8 periods)					*Under Construction*		
Focused	2.0	23	Double Crystal	4000–23000			
White Light Laue	0.5			4000–45000			
10-2 (15 periods)							6-circle Diffractometer
Focused	2.3	22	Double Crystal	2400–21000	$\sim5 \times 10^{-4}$	0.5 × 4.0	
Unfocused	1.0		Double Crystal	2400–40000	$\sim10^{-4}$	2.0 × 20.0	
10-2 Diffractometer							6-circle Diffractometer
11-2 (13 periods)					*Under Construction*		
Focused	~2	23	Double Crystal	4500–23000			
Unfocused	~1			4500–45000			
Side Stations							
4-1	1.0		Double Crystal	2400–35000	$\sim5 \times 10^{-4}$	2.0 × 20.0	
4-3							
Focused	1.0	Variable	Double Crystal	2400–15000	$\sim10^{-4}$	0.15 × 20.0	
Unfocused	1.0		Double Crystal	2400–35000	$\sim10^{-4}$	2.0 × 20.0	
7-1	1.0		Curved Crystal	6000–13000	$\sim8 \times 10^{-4}$	0.6 × 3.0	30 cm MAR Detector
7-3	1.0		Double Crystal	2400–35000	$\sim10^{-4}$	2.0 × 20.0	
9-1	3.0	16	Curved Crystal	11500–13500	*Under Construction*		30 cm MAR Detector
9-3					*Under Construction*		
Focused	2.5	23	Double Crystal	4600–23000			
Unfocused	0.7		Double Crystal	4600–40000			
VUV/SOFT X-RAY STATIONS							
5-2 multi-undulator	1.5		4 Gratings	10–1000	1×10^{-3}	$1 mm^2$	Circular Polarization
5-3 multi-undulator	1.5		4 Gratings	20–250	$1.0\text{–}2.0 \times 10^{-3}$	$\leq 1 mm^2$	
5-4			NIM		*Under Commisioning*		
10-1 wiggler side station	2.0		6m SGM	250–1200	$\sim2 \times 10^{-4}$	$\geq 0.1 mm^2$	
BEND MAGNET STATIONS							
X-RAY							
1-4	2.0		Curved Crystal	6700–10800	4.0×10^{-3}	0.25 × 1.0	SAXS Camera
1-5	1.0		Double Crystal	5500–30000	$\sim2 \times 10^{-4}$	2.0 × 17.0	CAD-4
1-5 ES2	1.0	14.5	Double Crystal	5500–14500	$\sim2 \times 10^{-4}$	$\leq 1 mm^2$	Fuji Imaging Plate
2-1 (Focused)	4.8	8.9	Double Crystal	2400–8900	$\sim5 \times 10^{-4}$	2.0 × 6.0	
2-2	1.0		None	3200–40000		4.0 × 22.0	
2-3	1.0		Double Crystal	2400–30000	$\sim5 \times 10^{-4}$	2.0 × 20.0	
VUV/SOFT X-RAY							
1-1	2.0		Grasshopper	24–1000	Δλ = .05–2Å	1.0 × 1.0	Commissioning
1-2	4.0		6m TGM	8–180	$\sim1 \times 10^{-3}$	0.1 × 0.5	
3-3	8–10	4.5	UHV Double Crystal	800–4500	$\sim5 \times 10^{-4}$	1.5 × 2.5	
3-4	0.6		Multilayer	0–3000	White or Δλλ = .6%	2.0 × 8.0	Vacuum Diffractometer Litho. Expo. Station
8-1	12		6m TGM	8–180	$\sim1 \times 10^{-3}$	$\geq 0.1 mm^2$	
8-2	5.0		6m SGM	150–1000	$\sim1 \times 10^{-4}$	$\geq 0.1 mm^2$	Circular Polarization

ADVANCED LIGHT SOURCE

University of California
Lawrence Berkeley National Laboratory
Berkeley, CA 94720

The Advanced Light Source (ALS) is a third-generation synchrotron source of high-brightness soft X-ray and ultraviolet radiation operated by the Lawrence Berkeley National Laboratory (LBNL) of the University of California.

Construction began in October 1987 and was completed in April 1993. The ALS is based on a low-emittance electron storage ring with 10 long straight sections available for insertion devices and 33 bend-magnet ports. The storage ring operates in the energy range from 1.0 to 1.9 GeV. The spectrum of synchrotron radiation depends on the radiation source and on the storage-ring energy. The brightest sources at the ALS are undulators placed in the straight sections of the storage ring. Undulators emit ultrabright laser-like beams that are highly focused in narrow wavelength bands. Existing undulator beamlines at the ALS provide high-brightness radiation at photon energies from below 10 eV to about 1.5 keV. A second type of insertion device, the wiggler, can access the hard X-ray region by generating broad-band radiation to about 20 keV. Bend magnets provide broad-band radiation to about 10 keV. Circularly polarized radiation is available from bend magnets and will be available from elliptical undulators. Infrared radiation will also be available from bend magnets. In the normal multibunch operating mode, the time structure of the radiation comprises pulses with a full-width-half-maximum of about 30 ps and separation between pulses of 2 ns; a two-bunch mode with maximum pulse separation of 656 ns is also provided on user request.

The ALS research program is extensive and steadily growing. The high brightness is opening new areas of research from the materials sciences, such as spatially resolved spectroscopy (spectromicroscopy), to the life sciences, such as X-ray microscopy with element-specific sensitivity. The scientific and technological impact of spatial resolution is extremely wide owing to the relentlessly decreasing size of the physical, chemical, and biological systems to be analyzed. Other beneficiaries of high brightness include very-high-resolution spectroscopy, spectroscopy of dilute species, spectroscopy and imaging of magnetic materials using circularly polarized radiation, diffraction from very small samples, and time-resolved spectroscopy and diffraction. Chemical analysis of semiconductor microstructures, X-ray crystallography of biological macromolecules for rational pharmaceutical design, at-wavelength interferometric testing of X-ray optical elements for future projection lithography systems, X-ray metrology, and microstructure fabrication by the LIGA process using proximity X-ray lithography are example of research programs with direct industrial interest and participation. The table summarizes existing experimental facilities and those planned for installation through 1998.

USER MODE

The ALS operates year around with scheduled shutdowns for installation of new experimental facilities and for accelerator maintenance. The current operating schedule provides 16 shifts per week for users (1 shift = 8 hours). As a national user facility, the ALS is available without charge to personnel from university, industrial, and government laboratories for non-proprietary research intended for publication in the open literature. Proprietary research is also welcome but is subject to a cost-recovery charge for provision of beam time. Proprietary users have the option to take title to any inventions made during the proprietary research program and treat as confidential all technical data generated during the program.

Whether non-proprietary or proprietary, there are two primary modes of conducting research at the ALS: as a member of a participating research team (PRT) or as an independent investigator. PRTs are collaborative groups comprising research personnel from one or more institutions with common research interests who contribute to the construction, operation, and maintenance of experimental facilities (beamlines and experimental stations) at the ALS for this purpose. In return for their contributions, PRT members are granted priority for a percentage of the operating time on their facilities. The remaining operating time on each beamline is allotted to scientists who are not members of a PRT (independent investigators). The proportion of time available to independent investigators varies from beamline to beamline. Independent investigators may bring their own experimental stations to ALS beamlines. Proposals for the establishment of new PRTs are reviewed by the Program Advisory Committee. Proposals for beam time from independent investigators are peer-reviewed by the Proposal Study Panel twice a year with 1 June and 1 December deadlines for receipt of proposals. For details, consult the ALS Users' Handbook, which is available from the Program Administrator at the address below. A safety handbook, an beamline design guide, and an annual activity report describing the previous year's accomplishments is also available.

PERSON TO CONTACT FOR INFORMATION

Elizabeth Saucier, Program Administrator	(510) 486-6166
Advanced Light Source	Fax (510) 486-4960
Lawrence Berkeley National Laboratory	E-mail: ECSaucier@lbl.gov
MS 80-101	
Berkeley, CA 94611	

SUMMARY OF ALS EXPERIMENTAL FACILITIES

The ALS complement of experimental facilities (insertion devices, beamlines, and experimental stations) continues to grow as new research opportunities become defined and funding becomes available. Experimental facilities are developed and operated by participating research teams working with the ALS staff. The table lists existing beamlines and beamlines planned through 1998 for which funding is available. Beamline designations X.Y.Z refer to storage ring sector number X, port number Y, and branch number Z. A fourth digit is used for fixed experimental stations with substantially different programs. There are 12 sectors. Ports 0 are insertion-device ports, ten of which are available for insertion devices; ports 1, 2, 3, and 4 are bend-magnet ports. Each branch may service multiple experimental stations. EPU is an elliptically polarizing undulator.

Beamlines available at the Advanced Light Source through 1998.

Beamline Number	Radiation Source	Scientific Program	Spectral Range	When Available
BTF	ALS linac	Beam Test Facility	50 MeV elec.	Now
1.4	Bend magnet	Infrared spectromicrscopy, surface science, pump-probe experiments	0.05-1 eV	Now
3.1	Bend magnet	Diagnostic beamline	200-280 eV	Now
4.0-1-2	EPU	Magnetic spectroscopy	100-2000eV	1998
4.0.3-4	EPU	Magnetic microscopy	100-1600eV	1998
5.0.1	Wiggler	Monochromatic protein crystallography	7-14 keV	1998
5.0.2	Wiggler	Multiple-wavelength (MAD) and monochromatic protein crystallography	3.5-14keV	Now
5.3.1	Bend magnet	Scanning transmission X-ray microscopy	250-750eV	1998
6.1.2	Bend magnet	High-resolution zone-plate microscopy	500-800eV	Now
6.3.1	Bend magnet	Calibration and standards, EUV/soft X-ray optics testing, solid-state chemistry	100-2000eV	1998
6.3.2	Bend magnet	Calibration and standards; EUV optics testing; atomic, molecular, and materials science	50-1300eV	Now
7.0.1	Undulator	Surface and materials science, spectromicroscopy, spin resolution, photon-polarization dichroism	60-1000eV	Now
7.0.2	Undulator	Coherent optics experiments	70-650eV	1997
7.2	Bend magnet	Deep-etch X-ray lithography (LIGA)	3-12keV	1998
7.3.1.1	Bend magnet	Magnetic spectromicroscopy	260-1500keV	1997
7.3.1.2	Bend magnet	Surface and materials science, micro X-ray photoelectron spectroscopy	260-1500eV	Now
7.3.3	Bend magnet	X-ray microdiffraction, X-ray absorption spectroscopy, sub-picosecond time-resolved X-ray diffraction	3-12keV	1997
8.0.1	Undulator	Surface and materials science, spectromicroscopy, imaging photoelectron spectroscopy	60-1000eV	Now

9.0.1	Undulator	Atomic, molecular, and optical physics; high-resolution gas-phase spectroscopy*	20-320eV	Now
9.0.2.1	Undulator	Chemical reaction dynamics, photochemistry	5-30eV	Now
9.0.2.2	Undulator	Photoionization spectroscopy and dynamics	5-30eV	Now
9.3.1	Bend magnet	Atomic, molecular, and materials science	2.2-6keV	Now
9.3.2	Bend magnet	Chemical and materials science, photon polarization dichroism	30-1500eV	Now
10.0.1*	Undulator	High-resolution atomic, molecular, and optical physics; photoemission of highly correlated materials	20-320eV	1998
10.3.1	Bend magnet	X-ray fluorescence microprobe	3-20keV	Now
10.3.2	Bend magnet	X-ray optics development, deep-etch X-ray lithography (LIGA), materials science	3-12keV	Now
11.3	Bend magnet	EUV lithography	50-1300eV	1998
12.0.1.1	Undulator	Surface and materials science, spectromicroscopy	60-320eV	Now
12.0.1.2	Undulator	EUV lithography optics testing, interferometry	60-320eV	Now

*The atomic and molecular science beamline will move to 10.0.1 in early 1998.

SECTION F

Other User Facilities

MATERIALS PREPARATION CENTER

Ames Laboratory
Iowa State University
Ames, Iowa 50011

The Materials Preparation Center was established because of the unique capabilities for preparation, purification, fabrication and characterization of certain metals and materials that have been developed by investigators at the Ames Laboratory during the course of their basic research. Individuals within the Laboratory's Metallurgy and Ceramics Program are widely recognized for their work with very pure rare-earth, alkaline-earth and refractory metals. Besides strengthening materials research and development at the Ames Laboratory, the Center increases awareness by the research community of the scope and accessibility of this resource to universities, other government and private laboratories and provides appropriate transfer of unique technologies developed at the Center to private, commercial organizations. The Center is presently upgrading its equipment pool through support of the Scientific Facilities Initiative.

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 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.

In addition to a Materials Preparation Section, the Center also consists of 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, selected services of this section are available to the research community. The purpose of MRSH is to accumulate information from a wide range of commercial and National Laboratory sources regarding the preparation and characterization of materials and to make this information available to the scientific community. The High-T_c Superconductivity Information Exchange provides a centralized site for rapid dissemination of up-to-date information on high-temperature superconductivity research. It publishes the newsletter, High-T_c Update, twice-monthly without charge, as both hard copy and electronic mail.

USER MODE

Materials Preparation and Analytical Sections

Quantities of ultrapure rare-earth metals and alloys in single and polycrystalline forms are available. Special preparations of high-purity oxides and compounds are also available in limited quantities. Unique technologies developed at Ames Laboratory are used to prepare refractory metals in single and polycrystalline forms. In addition, certain alkaline-earth metals used as reducing agents are available. Complete characterization of these materials are provided by the Analytical Section. Materials availability and characterization information can be obtained from Lawrence L. Jones, Director, Materials Preparation Center or Thomas A. Lograsso, MRSH Manager.

Materials Referral System and Hotline

The services of the Materials Referral System are available to the scientific community and inquiries should be directed to Thomas A. Lograsso, MRSH Manager, (515) 294-8900.

High-T_c Superconductivity Information Exchange

The newsletter, High-T_c Update, is published twice-monthly and available without charge as either hard copy or electronic mail. Inquiries should be directed to Sreeparna Mitra, (515) 294-3877.

MATERIALS PREPARATION CENTER (continued)

TECHNICAL DATA

MATERIALS

Scandium	Titanium	Magnesium	Thorium
Yttrium	Vanadium	Calcium	Uranium
Lanthanum	Chromium	Strontium	
Cerium	Manganese	Barium	
Praseodymium	Zirconium		
Neodymium	Niobium		
Samarium	Molybdenum		
Europium	Hafnium		
Gadolinium	Tantalum		
Terbium	Tungsten		
Dysprosium	Rhenium		
Holmium			
Erbium			
Thulium			
Ytterbium			
Lutetium			

PERSON TO CONTACT FOR INFORMATION

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

Thomas A. Lograsso, Associate Director (515) 294-8900
Ames Laboratory
Materials Preparation Center
109 Metals Development Building
Ames, IA 50011

ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH

Argonne National Laboratory
Argonne, Illinois 60439

The Argonne National Laboratory Electron Microscopy Center for Materials Research provides unique facilities which combine the techniques of high-voltage electron microscopy, ion-beam modification, and ion-beam analysis, along with analytical electron microscopy.

The HVEM-Tandem Accelerator Facility, which combines two microscopes and two ion accelerators, is the cornerstone of the Center. A High Voltage Electron Microscope (HVEM: a 1.2 MeV Kratos/AEI EM7) and a recently installed intermediate Voltage Electron Microscope (IVEM: a 300 kV Hitachi 9000 NAR) are interfaced to either of two ion accelerators, a 650 kV NEC implanter and a 2 MeV NEC Tandem accelerator. Ion beams of most stable elements, with energies from 10 keV to 8 MeV, can be transported into the HVEM or IVEM to permit direct observation of the effects of ion and/or electron bombardment of materials. Additionally, the HVEM and IVEM have 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 and PEELS. VG603Z advanced Analytical Electron Microscope (AEM) is now available for collaborative research. This field emission gun ultra-high vacuum AEM operates up to 300 keV and has excellent microanalytical capabilities for XEDS, EELS, and Auger Electron Spectroscopy AES.

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 either of the persons named below. Proposals are peer reviewed by a Steering Committee composed of ANL and non-ANL scientists. There are no use charges for non-proprietary research of documented interest to DOE. Use charges will be levied for proprietary investigations.

PERSON(S) TO CONTACT FOR INFORMATION

C. W. Allen (630) 252-4157
and
E. A. Ryan (630) 252-5222
Electron Microscopy Center for Materials Res.
Materials Science Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439

ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH (continued)

TECHNICAL DATA

ELECTRON MICROSCOPES	KEY FEATURES
High-Voltage Electron Microscope Kratos/AEI EM7 (1.2 MeV)	Resolution 9 Å pt-pt Continuous voltage selection Current density 15 A/cm^2 High-vacuum specimen chamber Electron and ion dosimetry systems Video recording system Ion-beam interface Specimen stages 10 - 1300 K Straining and environmental stages
Transmission Electron Microscope Hitachi H-9000 NAR (300 keV)	Resolution 2.5Å pt-pt Ion beam interface Specimen holders (15- 1200 K)
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, PEELS, video 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 VG603Z (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 Tandem	Terminal voltage 2 MV Energy stability ± 250 eV Current density: H^+, 10 μA/cm^2 (typical) Ni^+, 3 μA/cm^2
NEC 650 kV Ion Implanter	Terminal voltage 650 kV Energy stability ± 60 eV Current density: He^+, 100 μA/cm^2 (typical) Ar^+, 10 μA/cm^2

CENTER FOR MICROANALYSIS OF MATERIALS

Frederick Seitz Materials Research Laboratory
University of Illinois
Urbana-Champaign, Illinois 61801

The Center operates a wide range of advanced microchemistry, surface chemistry, electron microscopy, X-ray and electron-beam microanalytical equipment for the benefit of the University of Illinois materials research community and for the DOE Laboratories and Universities Programs. Equipment is selected to provide a spectrum of advanced microcharacterization techniques including microchemistry, micro-crystallography, surface analysis, structure determination, etc. A team of professionals runs the facility and facilitates the research.

USER MODE

Most of the research in the facility is funded from the MRL, DOE, and NSF contracts, and is carried out by graduate students, post-doctoral and faculty researchers and by the Center's own professional staff. The Center welcomes external users from national laboratories, universities, and industry.

For the benefit of external users the system retains as much flexibility as possible. The preferred form of external usage is collaborative research with a faculty member associated with the MRL. Independent usage by trained individuals is also encouraged. Assistance and collaboration with the professional staff of the Center is arranged as required. In all cases, the research carried out by users of the Center has to be in the furtherance of DOE objectives.

The equipment is made available on a flexible schedule. Professional help by the Center staff will be arranged to assist the users. Fully qualified users can and do use the equipment at any time of the day.

The Center staff maintain training programs in the use of the equipment and teach associated techniques. Part of the Center's activity is concerned with the development of new instruments and instrumentation.

In addition to the main items listed opposite, the Center also has other equipment: optical microscopes, a surface profiler, a microhardness tester, etc. Dark rooms and full specimen preparation facilities are available, including ion-milling stations, a micro-ion mill, electropolishing units, sputter coaters, a spark cutter, ultrasonic cutter, diamond saw, dimpler, etc.

PERSON TO CONTACT FOR INFORMATION

Dr. J. A. Eades, Coordinator (217) 333-8396
Center for Microanalysis of Materials
Materials Research Laboratory
University of Illinois Frederick Seitz
104 S. Goodwin
Urbana, IL 61801

See the CMM Homepage at: http://www.mrl.uiuc.edu/~cmm/index.html

CENTER FOR MICROANALYSIS OF MATERIALS (continued)

INSTRUMENTS CHARACTERISTICS	"ACRONYM"	FEATURES AND
Imaging Secondary Ion Microprobe Cameca IMS 5f	SIMS	Dual ion sources (Cs^+, O_2^+). 1 µm resolution.
Scanning Auger Microprobe Physical Electronics 660	Auger	Resolution: SEM 25 nm Auger 60 nm
X-ray Photoelectron Spectrometer Electronics 5400	XPS	Resolution: 50 meV, 180° Physical spherical analyzer, Mg/Al and Mg/Ag anodes
X-ray Photoelectron Spectrometer Surface Science	XPS	Spherical analyzer, small spot size, gas doping, high temperature
Transmission Electron Microscope Philips EM420 (120kV) Stage (30K).	TEM	EDS, EELS, STEM, Cathodoluminescence,
Transmission Electron Microscope Philips EM400T (120kV)	TEM	EDS. Heating, cooling stages
Transmission Electron Microscope Philips CM12 (120 kV)	TEM	EDS, STEM, Heating, cooling stages
Transmission Electron Microscope JEOL 4000EX (400 kV)	TEM	For environmental cell use. Straining stages, heating stages
Transmission Electron Microscope Hitachi 9000 (300 kV)	TEM	0.19nm resolution atomic imaging
Scanning Transmission E.M. Vacuum Generators HB501 (100kV)	STEM	0.5 nm probe, field emission gun, EDS, EELS (on order)
Scanning Electron Microscope Hitachi S800	SEM	Field Emission Gun Resolution 2 nm, EDX
Scanning Electron Microscope Zeiss 960	SEM	Backscattering (EBSP), EDX, Cathodoluminescence, Helium Stage
Scanning Tunnelling Microscope Omicron VT	STM	Variable temperature 30K - 1000K Auger, gas dosing, ion cleaning

CENTER FOR MICROANALYSIS OF MATERIALS (continued)

INSTRUMENTS CHARACTERISTICS	"ACRONYM"	FEATURES AND
X-ray Equipment Enraf-Nonius 18kW source Elliott 14 kW source Rigaku 12 kW source Several conventional sources Rigaku D/Max-11B Computer Controlled Powder Diffractometer Scintag diffractometers(2)	X-ray	4-circle diffractometer. Bede high-precision diffractometer 3-circle diffratometer Powder cameras, etc. High temperature and low temperature stages. Texture analysis.
Van de Graff Accelerator for High Voltage Engineering 3 MeV Tandem Accelerator general ionex 1.7 MeV	RBS etc.	Rutherford Backscattering ion irradiation and implantation PIXE Proton Induce X-ray Emission)
Low-energy electron microscopy (Tromp-IBM)	LEEM	10-100 eV UHV surface analysis Surface structure crystal growth evaporation

NATIONAL CENTER FOR ELECTRON MICROSCOPY

Lawrence Berkeley National 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 National 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 1.5 MeV Kratos microscope dedicated largely to *in situ* work, a 1-MeV JEOL atomic resolution microscope (ARM) with 1.6 angstrom point-to-point resolution, a 200-kV high-resolution microscope (JEOL 200 CX), a 200-kV analytical microscope (JEOL 200 CX) equipped with a thin window and a high-angle X-ray detector, and a parallel energy-loss spectrometer; a 200 kV *in situ* microscope with an electrical biasing holding, a 200 kV field emission microscope with an imaging energy filter, and a 300 kV field emission microscope with imaging energy filter for ultrahigh resolution Facilities for computer image simulation, processing and analysis 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. D. G. Howitt, Chairman, C. W. Allen, D. J. Smith, R. Mishra and K. Downing; internal members are: Drs. G. Thomas, K. M. Krishnan, R. Gronsky, and K. H. Westmacott). A limited number of studies judged by the Steering Committee to be of sufficient merit can be carried out as a collaborative effort between a Center post-doctoral fellow, the outside proposer, and a member of the Center staff. The Center also provides access to junior faculty and researchers through an annual visiting scientist fellowship award.

PERSON TO CONTACT FOR INFORMATION

Ms. Gretchen Hermes (510) 486-5006
National Center for Electron Microscopy
Mail Stop: 72-150
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720

NATIONAL CENTER FOR ELECTRON MICROSCOPY (continued)

TECHNICAL DATA

INSTRUMENTS	KEY FEATURES	CHARACTERIZATION
KRATOS 1.5-MeV Electron Microscope	Resolution 3 Å (pt-pt) environmental cell; hot stage, cold stage, straining stage, straining/heating stage, CBED, video camera, Faraday cup	50-80 hrs/week 150-1500 kV range in 100 kV steps and continuously variable. LaB_6 filament. Max. beam current 70 amp/cm^2. 3-mm diameter specimens.
JEOL 1-MeV Atomic Resolution Microscope	Resolution < 1.6 Å (pt-pt) over full voltage range. Ultrahigh resolution goniometer stage, ±40° biaxial tilt with height control.	60 hrs/week, 400 kV-1 MeV, LaB_6 filament, 3-mm diameter specimens.
JEOL 200 CX Electron Microscope	Dedicated high-resolution 2.4 Å (pt-pt) U.H. resolution goniometer stage only.	200 kV only, LaB_6 filament, 2.3-mm or 3-mm diameter specimens.
JEOL 200 CX dedicated Analytical Electron Microscope	Microdiffraction, CBED, UTW X-ray detector, high-angle X-ray detector, PEELS spectrometer.	100 kV-200 kV LaB_6 filament, state-of-the-art resolution; 3-mm diameter specimens.
JEOL 200 CX Electron Microscope	In-situ instrument with electrical biasing holder, heating stage and video camera.	100 kV-200 kV LaB_6 filament; side entry stage; 3-mm diameter specimens.
Philips CM200 FEG Electron Microscope	Field emission microscope, 2.4Å (pt.-pt) resolution; holography; energy filter, video and CCD cameras, hot stage.	200kV FEG side entry, 5 axis compustage; 3mm diameter specimens.
Phillips CM 300 FEG Electron Microscope	Field emission microscope 1.7A (pt.-pt.) resolution 1.0A information Limit. Holography, energy filter, video And CLD cameras	300 kV FED side entry, 5 axis compustage, 3MM diameter specimens

SHARED RESEARCH EQUIPMENT PROGRAM (SHaRE)

Metals and Ceramics Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

A wide range of facilities for use in materials science are available for collaborative research between university, industry, and other government laboratory researchers and ORNL staff members. Facilities are available for state-of-the-art intermediate voltage electron microscopy, atom probe/field ion microscopy, scanning electron microscopy, atomic force microscopy, surface analysis, and nuclear microanalysis. The electron microscopy capabilities include analytical electron microscopy [energy dispersive X-ray spectrometry (EDS), electron energy-loss spectrometry (PEELS), energy-filtered transmission electron microscopy, spectrum imaging, and selected area and convergent beam electron diffraction (CBED)]. A high resolution FEG-SEM is equipped for automoated orientation imaging microscopy and light-element EDS, atom probe field ion microscopy facilities permit single atom analysis. Surface analysis facilities include three Auger electron spectroscopy (AES) systems, and 0.4, 2.5, and 4.0 MeV Van de Graaff accelerators for radiation effects studies and ion beam modification treatments. Other equipment includes two mechanical properties microprobes (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 ORISE, ORNL, and external personnel. Current members are: E. A. Kenik, Chairman, J. Bentley, M. L. McCartney, E. L. Hall, and N. D. Evans. Proposals are evaluated on the basis of scientific excellence and relevance to DOE needs and current ORNL research. One researcher at ORNL must be identified who is familiar with required techniques and will share responsibility for the project.

The SHaRE program provides limited travel and specimen preparation support for U.S.A. academic participants through the Oak Ridge Institute for Science and Education (ORISE).

PERSONS TO CONTACT FOR INFORMATION

E. A. Kenik
Metals and Ceramics Division
Oak Ridge National Laboratory
P. O. Box 2008
Oak Ridge, TN 37831
(423) 574-5066
email: kenikea@ornl.gov

N. D. Evans
Oak Ridge Institute for Science and Education
P. O. Box 117
Oak Ridge, TN 37831
(423) 576-4427
email: evansnd@ornl.gov

SHARED RESEARCH EQUIPMENT PROGRAM (SHaRE)

TECHNICAL DATA

Facilities	Key Capabilities	Applications
Philips CM12 AEM 120kV	EDS, CBED, STEM;*	Structural and elemental microanalysis
Phillips CM 200/ FEG AEM 200 kV	EDS, CBED, (P) EELS, STEM; minimum probe ~1 nm Spectrum imaging*	Structural and elemental microanalysis
Philips CM30 AEM 300 kV	EDS, (P) EELS, CBED, STEM; energy filter*	Structural and elemental microanalysis
Philips XL30/FEG Scanning Electron Microscope 30 kV	SEM, EDS (WDS), EBSP minimum probe ~1.5 nm	Structural and elemental analysis
Atom Probe Field-Ion microscopes	TOF atom probe, imaging atom probe, FIM, pulsed	Atomic resolution imaging: single atom analysis laser atom probe elemental mapping
PHI 590 Scanning Auger Electron Spectroscopy System	200 nm beam; fracture stagee; 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, 2.5 MV, 4 MeV Van de Graff accelerators sputter profiling	Nuclear microanalysis; Rutherford backscattering; elemental analysis
Mechanical Properties Microprobe-Nanoindenter	Computer-controlled diamond indenter, cooling/heating capability, scratch-testing	High spatial resolution (0.1 μm lateral and 0.2 nm depth) measurements of elastic/plastic and viscoelastic behavior
Park Autoprobe - XL Atomic Force Microscope	Optical-based position sensing, quantitative	Surface imaging; repulsive or attractive imaging modes.

* Video recording; stages for cooling, heating, and deformation available for Philips microscopes

SURFACE MODIFICATION AND CHARACTERIZATION RESEARCH CENTER

Solid State Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

Ion implantation doping, ion-induced mixing, ion beam deposition, and other ion beam based techniques are utilized to alter the near-surface properties of a wide range of solids under vacuum conditions. *In situ* analysis 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 process, 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, semiconducting and optoelectronic devices, superconductors, etc.

This program emphasizes long-range basic research. Consequently, most cooperative research involving scientists from industries, universities, and other laboratories has focused on the investigation of new materials properties possible with these processing techniques and on the determination of mechanisms responsible for the observed property changes. In many instances such research projects identify 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 that can effectively utilize the unique alteration/analysis capabilities of the SMAC facility. The goal of these interactions is to demonstrate the usefulness or feasibility of these techniques for a particular materials application. Routine service alterations or analyses are discouraged.

PERSON TO CONTACT FOR INFORMATION

D. B. Poker (423) 576-8827
Solid State Division
Oak Ridge National Laboratory
Oak Ridge, TN 37831-6048
dbp@ornl.gov

SURFACE MODIFICATION AND CHARACTERIZATION RESEARCH CENTER (continued)

TECHNICAL DATA

ACCELERATORS	OPERATING CHARACTERISTICS
2.5-MV positive ion Van de Graaff	0.1-2.5 MeV H, ^{4}He, ^{3}He, and selected gases. Beam current up to 100 μA
1.7-MV tandem	0.2-3.5 MeV H; 0.2-5.1 MeV ^{3}He, ^{4}He; rf gas source and sputtering source for up to MeV energy ion beams of most elements.
35-170-kV high-current ion implantation accelerator	Most ion species; 100-1000 microamps singly charged ions; factor of 10 less for doubly charged ions
10-500-kV high-current ion implantation accelerator	Most ion species from microamp to milliamp currents
FACILITIES	
UHV implantation and analysis chambers	Several chambers with vacuums 10^{-6}-10^{-11} Torr; multiple access ports; UHV goniometers with temperature range 4-1300 K
In-situ analysis capabilities	Ion scattering, ion channeling, and ion-induced nuclear reactions; PIXE; LEED Auger
Rapid thermal annealer	AG Heatpulse Model 410, with programmable, multistep heating to 1200°C.
Thermal annealer	Heating to 1200°C under flowing gas or Torr vacuum

SURFACE MODIFICATION AND CHARACTERIZATION RESEARCH CENTER (continued)

TECHNICAL DATA

ACCELERATORS	OPERATING CHARACTERISTICS
Computer	Data acquisition and reduction; ion implantation and ion backscattering simulation
4-Point Resistance Probe	VEECO FPP5000
Nanoindenter	Nanoinstruments Models IIs

COMBUSTION RESEARCH FACILITY - MATERIALS PROGRAM

Sandia National Laboratories
Livermore, California 94551-0969

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. sulfidizing environments.	Pulsed lasers gated detection for blackbody background rejection. Furnace allows exposure to oxidizing, reducing, and
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.

COMBUSTION RESEARCH FACILITY - MATERIALS PROGRAM (continued)

Sandia National Laboratories
Livermore, California 94551-0969

TECHNICAL DATA

INSTRUMENTS	KEY FEATURES	COMMENTS
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.

SUMMARY OF FUNDING LEVELS

During the Fiscal Year ending September 30, 1996, the Materials Sciences total support level amounted to about $341.9 million in operating funds (budget outlays) and $329.7 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)	30.3	19.4
(b) South.................. (AL, AR, FL, GA, KY, LA, MS, NC, SC, TN, VA, WV)	19.6	12.1
(c) Midwest................ (IA, IL, IN, MI, MN, MO, OH, WI)	19.0	40.1
(d) West................... (AZ, CO, KS, MT, NE, ND, NM, OK, SD, TX, UT, WY, AK, CA, HW, ID, NV, OR, WA)	31.1	28.4
	100.0	100.0

2. By Discipline:

	Grant Research (% by $)	Total Program (% by $)
(a) Metallurgy, Materials Science, Ceramics (Budget Activity Numbers 01-)	57.2	42.6
(b) Physics, Solid State Science, Solid State Physics (Budget Activity Numbers 02-)	33.2	27.0
(c) Materials Chemistry (Budget Activity Numbers 03-)	9.6	10.4
(d) Facility Operations	----	20.0
	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., LBNL, Ames and IL)	25.2
(b) DOE Laboratory Research Programs	29.3
(c) Major Facilities at DOE Laboratories	44.3
(d) Industry and Other	1.2
	100.0

4. By Laboratory and Grant Research:

	Total Program (%)
Ames Laboratory	3.3
Argonne National Laboratory	26.4
Brookhaven National Laboratory	19.6
Idaho National Engineering and Environmental Lab.	1.2
Illinois, University of (Frederick Seitz Materials Research Laboratory)	3.4
Lawrence Berkeley National Laboratory	3.3
Lawrence Livermore National Laboratory	1.2
Los Alamos National Laboratory	4.3
National Renewable Energy Laboratory	1.1
Oak Ridge National Laboratory	10.4
Pacific Northwest National Laboratory	1.2
Sandia National Laboratory	2.5
Stanford Synchrotron Radiation Laboratory	1.2
Grant Research	20.9
	100.0

SECTION H

Index of Investigators,

Materials, Techniques,

Phenomena, and Environment

INVESTIGATOR INDEX

MATERIALS, TECHNIQUES, AND PHENOMENA

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 1997 were $341,910,000. The number of projects is 517.

MATERIALS

Actinides-Metals, Alloys and Compounds
10, 15, 19, 38, 60, 147, 157, 167, 175, 176, 178, 203, 257, 280, 309, 320, 324, 373, 392, 420, 447
(0.86, 0.84, 3.85)

Aluminum and its Alloys
1, 7, 10, 24, 29, 33, 48, 58, 74, 78, 88, 125, 127, 130, 155, 157, 158, 165, 172, 183, 190, 194, 196, 197, 204, 212, 214, 227, 232, 240, 249, 263, 272, 341, 343, 360, 399, 417, 427, 435, 445, 508, 509, 527, 539, 544
(2.42, 1.29, 8.44)

Alkali and Alkaline Earth Metals and Alloys
3, 10, 48, 62, 67, 153, 155, 203, 306, 343, 431, 508
(0.46, 0.21, 2.20)

Amorphous State: Liquids
47, 63, 115, 120, 171, 224, 225, 229, 257, 269, 273, 297, 334, 336, 337, 429, 444, 479
(0.94, 0.36, 3.30)

Amorphous State: Metallic Glasses
22, 30, 76, 78, 93, 125, 171, 189, 198, 203, 212, 239, 246, 247, 257, 273, 286, 331, 337, 455
(0.86, 0.71, 3.67)

Amorphous State: Non-Metallic Glasses (other than Silicates)
35, 90, 97, 137, 167, 181, 206, 207, 210, 224, 246, 247, 257, 260, 261, 337, 348, 351, 391, 474
(0.72, 0.52, 3.67)

Amorphous State: Non-Metallic Glasses (Silicates)
20, 95, 229, 242, 257, 261, 262, 317, 322, 337, 348, 351, 448, 474, 524
(0.97, 0.39, 2.75)

Carbides
10, 20, 87, 90, 128, 142, 152, 205, 207, 218, 220, 228, 233, 261, 292, 295, 343, 418, 528, 536, 539, 542, 544
(1.14, 0.45, 4.22)

Cement and Concrete
408
(0.18, 0.03, 0.18)

Carbon and Graphite
48, 61, 137, 144, 153, 157, 169, 212, 218, 241, 396, 406, 431, 437
(0.57, 0.54, 2.57)

PHENOMENA

Divisions of the Office of Basic Energy Sciences

Divisions of the Office of Basic Energy Sciences are summarized below. Full program descriptions and research summary reports are available from each division.

Division of Chemical Sciences, Acting Director: Dr. William Millman, 301/903-5804.

The Chemical Sciences subprogram sponsors experimental and theoretical research on liquids, gases, plasmas, and solids. The focus is on their chemical properties and the interactions of their component molecules, atoms, ions, and electrons. The long-term goal is to contribute to new or improved processes for developing and using domestic energy resources in an efficient and environmentally acceptable manner.

Division of Energy Biosciences, Director: Dr. Gregory L. Dilworth, 301/903-2873.

Energy Biosciences sponsors research in the microbiological and botanical sciences. The research addresses the underlying mechanisms of green plant productivity by solar energy transformation, conversion of biomass and other organic materials into fuels and chemicals by novel and improved methods of fermentation, and biotechnologies capable of saving energy.

Division of Engineering and Geosciences, Acting Director: Dr. Iran L. Thomas, 301/903-3427

The **Engineering Research** activity sponsors research to strengthen the foundations of energy-related engineering practice aimed at long-term energy needs, while furthering advanced engineering education. Contact: Dr. Robert Price, 301/903-5822.

The **Geosciences Research** objectives include development of a knowledge base for predicting the behavior and response of geologic materials, such as rocks, minerals, and fluids, and the broader earth-sun system, to natural processes. Research areas include: fracture characteristics, fluid movement in geologic formations and reservoirs; indirect characterization and monitoring of geologic structures and *in situ* properties of rock masses.

Division of Materials Sciences, Director: Dr. Iran L. Thomas, 301/903-3427.

The Materials Sciences subprogram carries out basic research in materials science on strategic topics that are of critical concern to the mission and strategic plan of the Department of Energy. The subprogram is concerned with the fundamental scientific understanding and exploitation of the synergistic relationship between the synthesis, processing, structure, properties, behavior, and performance of materials including metals, ceramics, polymers, semiconductors, superconductors, and surfaces. The subprogram is also responsible for the operation of national user facilities and collaborative research centers involving synchrotron radiation, neutron sources, electron beam microcharacterization and the preparation of research quantities of special materials.