September 1986

Materials Sciences Programs
Fiscal Year 1986

U.S. Department of Energy
Office of Energy Research
Office of Basic Energy Sciences
Division of Materials Sciences
Washington, D.C. 20545
The Division of Materials Sciences is located within the Department of Energy in the Office of Basic Energy Sciences. The organizational structure of the Department of Energy is given in an accompanying chart. The Office of Basic Energy Sciences reports to the Director of the DOE Office of Energy Research. The Director of this Office is appointed by the President with Senate consent. The Director advises the Secretary on the physical research program; monitors the Department's R&D programs; advises the Secretary on management of the multipurpose laboratories under the jurisdiction of the Department, excluding laboratories that constitute part of the nuclear weapon complex; and advises the Secretary on basic and applied research activities of the Department.

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

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

This report contains a listing of research underway in FY 1986 together with a convenient index to the Division's programs. Recent publications from Division-sponsored panel meetings and workshops are listed on the next page.

Louis C. Ianniello, Acting Director
Division of Materials Sciences
Office of Basic Energy Sciences
RECENT DIVISION SPONSORED PUBLICATIONS

Topical and Workshop Reports

- Final Report the Workshop on Conductive Polymers (1985)
- Micromechanisms of Fracture (1985)
- Polymer Research at Synchrotron Radiation Sources (1985)
- Bonding and Adhesion at Interfaces (1985)
- Materials Preparation and Characterization Capabilities (1983)
- Critical and Strategic Materials (1983)
- Coatings and Surface Modifications (1983)
- High Pressure Science and Technology (1982)

Summary Research Bulletins (of Work in Progress)

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

Description of Research Facilities, Plans, and Associated Programs

- Centers for Collaborative Research
- Progress of the Office of Energy Research (1985)

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a Available in limited quantities from the Division of Materials Sciences.
b To be published.
c Also published in Materials Science and Engineering.
OFFICE OF BASIC ENERGY SCIENCES
Division of Materials Sciences Structure

Division of Materials Sciences

Acting Director: L. C. Ianniello
(Sandy Tucker-Secretary)
(301) 353-3427

Metallurgy and Ceramics Branch
Chief: F. V. Nolfi, Jr.
(Taree Thompson-Secretary)
(301) 353-3428
R. J. Gottschall
J. B. Darby
D. W. Keefer 1/

Solid State Physics and Materials Chemistry Branch
Chief: B. C. Frazer
(Kathy Rockenhauser-Secretary)
(301) 353-3426
T. A. Kitchens 2/
I. L. Thomas
J. E. Robinson 3/
W. T. Oosterhuis 4/
D. Liebenberg 5/

Notes:

1/ On Detail from Idaho National Engineering Laboratory (returned 9/86)
2/ Relocated to Applied Mathematical Sciences, DOE, 9/86
3/ On Detail from Argonne National Laboratory
4/ On Leave from National Science Foundation (returned to NSF 8/86)
5/ On Detail from Los Alamos National Laboratory
INTRODUCTION

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

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

Each project in Sections A, B, and C carries a number (at the left hand margin) for reference purposes, e.g., in Section G. The FY 1986 funding level, title, personnel, budget activity number (e.g., 01-2) and key words and phrases accompany the project number. The first two digits of the budget number refer to either Metallurgy and Ceramics (01), Solid State Physics (02), or Materials Chemistry (03). The budget numbers carry the following titles:

01-1 - Structure of Materials  
01-2 - Mechanical Properties  
01-3 - Physical Properties  
01-4 - Radiation Effects  
01-5 - Engineering Materials  
02-1 - Neutron Scattering  
02-2 - Experimental Research  
02-3 - Theoretical Research  
02-4 - Particle-Solid Interactions  
02-5 - Engineering Physics  
03-1 - Chemical Structure  
03-2 - Engineering Chemistry  
03-3 - High Temperature and Surface Chemistry

Sections D and E contain information on special DOE centers that are operated for collaborative research with outside participation. Section F summarizes the total funding level in a number of selected categories. Most projects have been classified under more than one category since the categories are not mutually exclusive. In Section G the references are to the project numbers appearing in Sections A, B, and C and are grouped by (1) investigators, (2) materials, (3) techniques, (4) phenomena, and (5) environment.

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

Preparation of this FY 1986 summary report was coordinated by I. L. Thomas. Though the effort required time by every member of the Division, much of the work was done by the Division's secretaries: S. Tucker, T. Thompson, and K Rockenhouser. Computer programming assistance was provided by S. Dorsey, Calculon, Inc.
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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.
Studies of interface structure and composition using Auger, ELS, and SIMS surface analytical techniques in combination with ion etching. Auger and reflection electron loss spectroscopy of metallic hydrides for phase identification and mapping. Effects of tin alloying on brass corrosion behavior in aqueous salt solutions. Scanning Auger microprobe analysis of effects of radiation on the competition between C and P grain boundary segregation in iron. Local chemical state information from Auger lineshape analysis in metallic glasses.

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

003. MICROSTRUCTURAL CONTROL IN METALS

Phone: (515) 294-9471
$580,000

Production of composite alloys by the in situ process and properties of in situ prepared Cu-base composite alloys. Problems in the diffusion of Sn and Ga to form Nb_2Sn and Nb_3Ga. Directional solidification studies on segregation and morphology in gray, nodular, and white cast iron. Evaluation of microstructural changes in the austempering of nodular cast irons. Microstructure evolution under solidification conditions typical of welding processes. Solidification processing of (Dy,Tb)Fe_2 magnetostrictive alloys. Processing and characterization of high coercivity, permanent magnet materials.

004. MECHANICAL METALLURGY

W. A. Spitzig, J. Kameda, A. Chatterjee
Phone: (515) 294-5082
$460,000

Effects of hydrogen on crack initiation in refractory alloys under uniaxial and cyclic loading conditions. Interstitial effects on strength and ductility in both nonhydrogenated and hydrogenated V, Nb, and Ta. Investigation of hydrogen diffusion in vanadium-base alloys by internal friction. Hydrogen-induced brittle cracking in both low and high hydrogen solubility bcc metals and alloys. Effects of radiation-induced defects and solute segregation on intergranular embrittlement. Modeling of hydrogen embrittlement. Description of three dimensional arrays of defects and relationship of arrangement to ductility and mechanical properties. Correlation between defect structure and nondestructive measurement.

005. STRUCTURE AND PROPERTY RELATIONS IN METALS

J. F. Smith
Phone: (515) 294-5083
$6579,000

006. TRANSPORT STUDIES

O. N. Carlson
Phone: (515) 294-2375
$135,000 01-3


007. HYDROGEN IN METALLIC SOLIDS

D. T. Peterson
Phone: (515) 294-6585
$170,000 01-3

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

008. RARE EARTH MATERIALS

K. A. Gschneidner Jr., K. Yagasaki
Phone: (515) 294-2272
$210,000 01-3

Quenching of spin fluctuations and other magnetic phenomena in: (1) highly enhanced paramagnets RCo$_2$ (R=Sc, Y and Lu), Sc and Pd-Ni alloys, (2) valence fluctuation materials CeSn$_x$ and CeSi$_x$ alloys, and (3) itinerant ferromagnets Sc$_3$In and ZrZn$_2$. Low-temperature, high-field heat capacity, magnetic susceptibility, electrical resistance and lattice parameters are used to characterize the behaviors. Nonequilibrium phases resulting from solidification and phase transformations in rare-earth-based alloys.
009. NDE MEASUREMENT TECHNIQUES

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

$552,000 01-5

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

010. ADVANCED MATERIALS AND PROCESSES

F. A. Schmidt, O. D. McMasters
Phone: (515) 294-5236 or (515) 294-1562

$189,000 01-5

011. NEUTRON SCATTERING

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

Study of the lattice dynamics, thermodynamic properties, and structural transformations of metals at high temperatures (bcc and fcc La), structure and diffusion in metal hydrides (ScHₓ, LaHₓ), dynamics and phase transitions of alkali-graphite intercalation compounds, electronic structure and phonon spectra of mixed valence compounds (CePd₃₋ₓ, Ce, YbAl₁₂), relation of electron-phonon interaction to superconductivity (La, CeSn₃). High pressure studies (-Ce, La). Study of the magnetic properties of heavy fermion superconductors (CeCu₂Si₂, UPt₃, UBe₁₃).

012. SEMICONDUCTOR PHYSICS

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

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

013. SUPERCONDUCTIVITY

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

Point contact Josephson effect in heavy fermion superconductors UBe₁₃, CeCu₂Si₂. Electron tunneling spectroscopy and surface physics studies of strong coupled transition metal superconductors. Proximity electron tunneling spectroscopy (PETS) of the electron-phonon spectrum F. Auger electron spectroscopy (AES), electron energy loss spectroscopy (ELS) and ultraviolet photoemission spectroscopy (UPS). Fundamental studies of superconductivity in metal-metal composites, use of Josephson junctions to study flux pinning of isolated vortices, development of materials with very low pinning, development of superconducting composites suitable for large scale magnets in the 8 to 16 Tesla range, practical studies to improve wire fabrication techniques, development of magnetic shielding devices, study of magnetostrictive materials.
014. OPTICAL AND SPECTROSCOPIC PROPERTIES OF SOLIDS AND LIQUIDS

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

$315,000 02-2

Electron photoemission and optical properties (transmission, reflection, ellipsometry, electroreflectance) of solids in the visible, vacuum ultraviolet and soft X-ray region using synchrotron radiation. Ce and Ce-compounds (e.g., CeSn₃) heavy Fermion systems, e.g., UPt₃, Fe-based alloys with Si and Al, benzotriazol on Cu, electroreflectance of emersed Ag electrodes, photon- and electron-stimulated desorption of neutral atoms from insulators.

015. NEW MATERIALS AND PHASES

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

$570,000 02-2

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

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

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

017. X-RAY DIFFRACTION PHYSICS

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

X-ray diffraction studies of semiconducting compounds, epitaxial layers, and superlattices as a function of the temperature. In-situ diffusion studies between layers in superlattices. X-ray studies of La at high pressures. X-ray Debye temperature and electron charge density studies of V₂Si and Fe-Ni-C in the vicinity of the martensitic phase transition. Active participation in the MATRIX PRT beam line at NSLS.

018. ELECTRONIC AND MAGNETIC PROPERTIES

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

AMES LABORATORY (continued)

019. OPTICAL AND SURFACE PHYSICS THEORY

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

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

020. SUPERCONDUCTIVITY THEORY

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


021. SYNTHESIS AND CHARACTERIZATION OF NEW MATERIALS

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

Synthesis, structure and bonding in intermetallic systems-new Zintl phases, new ternary compounds stabilized by interstitials. Reactions and stabilities of phases in the system CsI-Zr-ZrI4-ZrO2, effects of common impurities, the fate of the important fission products. Synthesis, structure and properties of new ternary oxide phases containing heavy transition elements, especially metal-metal bonded structures stable at high temperatures. Low temperature routes to new metal oxide, sulfide and nitride compounds. Correlation of structure and bonding with d-electron count and physical properties. Development of diffraction techniques for single crystal and non-single crystal specimens, techniques for pulsed-neutron and synchrotron radiation facilities, and use of Patterson superposition methods. Experimental methods include X-ray diffraction, photoelectron spectroscopy, resistivity and magnetic susceptibility measurements, high temperature reactions and synthesis of molecular precursors.
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AMES LABORATORY (continued)

022. CERAMIC MATERIALS

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

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

023. HIGH TEMPERATURE CHEMISTRY OF REFRACTORY MATERIALS

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

Study of refractory and corrosion-resistant materials such as transition
metal aluminides (Zr-Al, Ta-Al), phosphides and sulfides by both experi-
mental 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 transi-
tions. Experimental methods include X-ray and electron diffraction for
structure analysis, computer automated simultaneous mass loss-mass spectro-
metry for high temperature vaporization reactions related to stability, and
photoelectron spectroscopy for the electronic structure of solids. Elec-
tronic structure studies also include a program of band structure
calculations.
Evaluation of mechanisms of catalytic reactions, especially hydrogenation, hydrogenolysis, methanation, and hydrodesulfurization reactions, by surface characterization and kinetic techniques, with emphasis on single crystal and evaporated film catalysts. Study of lubrication phenomena: decomposition pathways and products of fluorinated organic molecules at surfaces. Mechanisms of corrosive oxidation of metals. Chemistry of electrode reactions, including electrocatalysis and corrosion reactions. Characterization of electrocatalytic materials by modulated hydrodynamic voltammetry. Reactivity of oxidized and doped electrode surfaces, including characterization of oxygen mobility and defect density at such electrodes. Surface chemistry of nucleation and flocculation applied to ceramic processing. Techniques used include low energy electron diffraction, Auger and scanning Auger electron spectroscopy, infra-red emission and electron energy loss spectrosopies, ring-disk and modulated hydrodynamic voltammetry.
A fundamental research program concerned with the atomic and electronic structure of defects in alloys and the relationship between these and the properties of stable and metastable phases and the nature of phase transformations. The research program involves investigations of defect properties and atomic and electronic structure in a variety of materials, with an emphasis on disordered and ordered alloy systems. These materials are being investigated with experimental techniques such as positron annihilation spectroscopy, Compton scattering, X-ray and neutron scattering, and transmission electron microscopy, along with complementary electronic structure calculations.

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

L. E. Rehn, R. S. Averback, R. C. Birtcher, M. A. Kirk, N. Q. Lam,
B. A. Loomis, P. R. Okamoto, H. Hahn, F.-R. Ding, A. Liu
Phone: (312) 972-5021
$1,268,000 01-4

Investigations of mechanisms leading to the formation of defect aggregates,
precipitates, and other inhomogeneous distributions of atoms in solids with
and without displacement-producing irradiation. Surface layer modification
of alloys by ion implantation, ion-beam mixing, and sputtering. Radiation-
induced segregation to internal and external defect sinks. Radiation-
enhanced diffusion. Effects of irradiation on alloy composition,
microstructure, and amorphization. In-situ studies of ion and electron
bombardment in the High-Voltage Electron Microscope. Neutron and dual-beam
ion irradiation. Computer modeling of irradiation-induced microstructural
changes. Ion-beam analysis. Analytical electron microscopy. Radiation
sources include HVEM-2MV Tandem facility and two 300-kV ion accelerators.

043. ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH

H. Wiedersich, C. W. Allen, A. Taylor, N. J. Zaluzec
Phone: (312) 972-5079
$1,329,000 01-4

Development and use of high-voltage and high-spatial resolution analytical
microscopy for materials research. Operation and development of the
Center's 1.2 MeV High-Voltage Electron Microscope-Tandem Facility with in-
situ capability for direct observation of ion-solid interactions. The HVEM
is currently being utilized for research programs in advanced materials,
mechanical properties, irradiation effects, oxidation and hydrogenation
effects. HVEM specimen stages are available for heating (1300 K), cooling
(10 K), straining, and gaseous environments. Ion-beam interface with 300 kV
ion accelerator and 2 MV tandem accelerator available for in-situ implanta-
tions and irradiations. A 600 kV ion accelerator is being procured as a
replacement for the 300 kV instrument. Approximately 50% of HVEM usage is
by non-ANL scientists on research proposals approved by the Steering
Committee for the Center that meets every six months. A state-of-the-art,
medium-voltage, ultra-high vacuum, field-emission gun, Analytical Electron
Microscope is being procured. Its design is directed toward the attainment
of the highest microanalytical resolution and sensitivity. Fundamental
studies of electron-solid interactions and microcharacterization of materials,
using TEM, STEM, XEDS, and EELS are conducted at present on lower-voltage
conventional electron microscopes.
ARGONNE NATIONAL LABORATORY (continued)

044. OXIDATION STUDIES

D. J. Lam, D. J. Baxter, W. E. King, K. Natesan, S. J. Rothman
Phone: (312) 972-4966
$763,000 01-5

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

045. AMORPHOUS METALLIC ALLOYS

P. R. Okamoto, R. S. Averback, T. I. Morrison, H. Hahn
Phone: (312) 972-5052
$581,000 01-5

ARGONNE NATIONAL LABORATORY (continued)

Intense Pulsed Neutron Source Division

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

046. INTENSE PULSED NEUTRON SOURCE PROGRAM

Phone: (312) 972-5518
$4,762,000 02-1

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

Solid State Physics - 02 -

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

047. NEUTRON AND X-RAY SCATTERING

Phone: (312) 972-5475
$1,726,000 02-1

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

048. SUPERCONDUCTIVITY AND MAGNETISM

B. D. Dunlap, G. W. Crabtree, K. E. Gray, D. G. Hinks,
H. A. Kierstead, T. I. Morrison, G. K. Shenoy, E. Alp, A. J. Fedro,
S. K. Malik, P. A. Montano, B. D. Terris
Phone: (312) 972-5538
$1,312,000 02-2


049. ELECTRONIC STRUCTURE AND BONDING

D. J. Lam, A. T. Aldred, S.-K. Chan, M. V. Nevitt,
B. W. Veal
Phone: (312) 972-4966
$897,000 02-2

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

050. LAYERED AND THIN FILM MATERIALS

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

$697,000 02-2

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

051. SYNCHROTRON RADIATION STUDIES

Phone: (312) 972-5537

$985,000 02-2

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

052. LOW DIMENSIONAL AND INTERFACE MATERIALS

Phone: (312) 972-5469
$307,000 02-2

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

053. 6GeV SYNCHROTRON SOURCE RESEARCH AND DEVELOPMENT

Y. Cho
Phone: (312) 972-6616
$834,000 02-2

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

054. CONDENSED MATTER THEORY

Phone: (312) 972-5507
$900,000 02-3

055. MODELING AND THEORY OF INTERFACES

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

$161,000 02-3

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

056. ULTRA-HIGH FIELD SUPERCONDUCTORS

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

$298,000 02-5

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

J. M. Williams, M. A. Beno, C. D. Carlson, A. J. Schultz,
Phone: (312) 972-3464

$2,010,000 03-1

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

058. THERMODYNAMICS OF ORDERED AND METASTABLE MATERIALS

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

$501,000 03-2

Experimental and theoretical investigations of important thermodynamic and
structural properties of ordered and associated solutions and amorphous
(metastable) materials. Thermodynamic and structural measurements (e.g.,
emf, vapor pressure, neutron diffraction) are combined with theoretical
calculations (e.g., molecular dynamics, statistical mechanics) to determine
the fundamental characteristics of ordered and associated solutions (e.g.,
chloroaluminates, ionic alloys, silicates). Other techniques such as small
angle neutron scattering, and inelastic neutron scattering are used to obtain
data relating to valence states, ordering and clustering of atoms and ions in
solution. The extension of our theories and concepts for pyrometallurgy
is explored.
059. INTERFACIAL MATERIALS CHEMISTRY
Phone: (312) 972-3513
$626,000 03-2

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

060. AQUEOUS CORROSION
Phone: (312) 972-3513
$628,000 03-2

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


Phone: (312) 972-3513

$883,000 03-3

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

Phone: (FTS) 666-3517 or 516-282-3517
$482,000 01-1

Experimental and theoretical studies of the fundamental factors which influence the adherence, integrity, stability, and other properties of surface layers of materials which have been modified by various means to have properties different from those within the bulk of the material, e.g., the interface between a coating and a substrate and grain boundaries in intermetallic compounds such as Ni$_3$Al. Research emphasizes microstructural and chemical characterization and the relation of these characteristics to physical and metallurgical properties using techniques such as glancing angle X-ray reflection and absorption, photoemission, positron annihilation, and transmission electron microscopy.

071. MECHANISMS OF METAL-ENVIRONMENT INTERACTIONS

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

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

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

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

073. PHYSICAL PROPERTIES OF METAL-INTERSTITIAL SYSTEMS

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

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

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

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

Solid State Physics - 02 -

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

075. MAGNETIC AND STRUCTURAL PHASE TRANSITIONS

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

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

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

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

077. EXPERIMENTAL RESEARCH - X-RAY SCATTERING

Phone: (FTS) 666-3821 or (516) 282-3821
$1,000,000 02-2

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

078. LOW ENERGY - PARTICLE INVESTIGATIONS OF SOLIDS

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

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

079. STRUCTURAL CHARACTERIZATION OF MATERIALS USING POWDER DIFFRACTION TECHNIQUES

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


080. THEORETICAL RESEARCH

Phone: (FTS) 666-3798 or (516) 282-3798
$840,000

Phase transitions, critical and cooperative phenomena in magnetic systems, organic metals and incommensurate structures, properties of one- and two-dimensional materials by analytical and numerical methods, nonlinear systems, metal surfaces and adsorbed films, surface states, electronic structure of metals and alloys, X-ray and neutron scattering, photoemission and inverse photoemission, properties of disordered materials and crystal defect physics, high pressure, high temperature properties of solids.
Synchrotron Radiation as a technique to study the geometrical and electronic properties of surfaces and interfaces. The use of new spectroscopies such as inverse photoemission, and the construction of an undulator beam line at the NSLS to enable spin polarized photoemission experiments for studies of the magnetic properties of surfaces. Support has also been given to the development of low-temperature techniques which can be used at the NSLS. The problems presently being studied include: a) electronic properties of overlayers, clean metal surfaces and interfaces; valence band photoemission, inverse photoemission and core level spectroscopy are used as tools in this area, b) organic molecules on surfaces and properties of organic solids, c) surface metallurgy and surface compounds, d) cooperative effects and phase transitions in adsorbate layers on metal surfaces, e) studies of metal clusters in rare gases and in organic solids, f) studies of oxidation and other chemical reactions at low temperatures.
The objective of this program is to support operations and development of the National Synchrotron Light Source (NSLS). The operations aspect covers operation and maintenance of the two NSLS electron storage rings and the associated injector combination of linear accelerator-booster synchrotron, operation and maintenance of the photon beam lines of the vacuum ultraviolet (VUV) and X-ray storage rings, and the technical support of experimental users. The development of the NSLS encompasses the further improvement of the storage rings to achieve maximum brightness photon sources and the further development of the photon beam lines of the facility by means of new developments in high resolution photon optics, state-of-the art monochromators, X-ray mirror systems, detectors, and so on. The NSLS storage rings provide extremely bright photon sources, several orders of magnitude more intense in the VUV and X-ray regions than conventional sources. While the original design has been solidly based on well developed principles of accelerator technology, this facility is the first in this country to be designed expressly for use of synchrotron radiation, and the objectives in machine performance are quite different from those of importance in high energy physics applications. An extensive research and development program is, therefore, necessary in order to optimize performance characteristics and also to develop new beam line instrumentation which will permit users to take full advantage of the unique research capabilities offered by this facility. This research and development (R&D) effort also supports the construction of the beam lines and devices funded under the Phase II construction project.
084. SYNTHESIS AND STRUCTURES OF NEW CONDUCTING POLYMERS

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

Development of a fundamental understanding of ionically and electronically conducting polymers. Research consists of the synthesis of new conducting polymers, the exploration of their physical properties, and the structural characterization by X-ray and neutron diffraction, electron microscopy, magnetic susceptibility, and electrical resistivity measurements. Also included are theoretical studies of the electronic structure and phase transitions of low-dimensional solids and the charge-transfer properties of new conducting polymers. The materials of interest are linear polyethers, polypyrrole, polysilane, etc. This is a collaborative program between Brookhaven National Laboratory and the Polytechnic Institute of New York.
Establishment of quantitative relationships between materials and processes used to weld them. Emphasis on predicting structure and properties of a weldment from process parameters and materials chemistry. Solidification and microstructure/properties correlations utilizing infrared thermography, moire interferometry, high-speed X-radiography, optical and electron microscopy, calorimetry, and computer modeling. Technology transfer through American Welding Institute.
105. EFFECT OF TRANSPORT PROCESSES ON LOCALIZED CORROSION

R. C. Alkire
Phone: (217) 333-3640

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

106. CENTER FOR MICROANALYSIS OF MATERIALS

J. A. Eades, C. Loxton, J. Woodhouse
Phone: (217) 333-8396, (217) 333-0386, or (217) 333-3888

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

107. RAPID SOLIDIFICATION PROCESSING

H. L. Fraser
Phone: (217) 333-1975

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

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

$130,000 01-1

Mechanisms and kinetics of crystal growth. Metastable single crystal alloys for solar and optical applications. Ion-beam sputtering, molecular-beam epitaxy, laser heating and low-energy ion bombardment methods applied to III-V based compounds and III-IV-V\textsubscript{2} chalcopyrite systems.

109. PROCESSING AND CHARACTERIZATION OF NOVEL AMORPHOUS MATERIALS AND SURFACES

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

$30,000 01-1

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

110. MICROCHEMISTRY OF SOLIDS

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

$65,000 01-1

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

111. PROCESSING AND MICROSTRUCTURE OF COMPLEX CERAMIC SYSTEMS

A. Zangvil
Phone: (217) 333-6829

$100,000 01-1

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

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

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

113. MICROMECHANICS AND MICROMECHANISMS OF FRACTURE

Phone: (217) 333-1901

Fracture mechanics and microstructural studies of the fundamental mechanisms of fracture are applied to metals and ceramics. Environmental effects on the fracture of alloys of Fe, Ni, Al, Ti, Al₂O₃-ZrO₂, MgO using HVEM. Role of phase transitions in fracture of hydride forming systems and stainless steels. Effects of environment on dislocation behavior and plasticity related fracture. High-temperature corrosion and scaling. Fatigue and fracture under multiaxial loading and the role of microstructural changes. Development of damage and failure criteria for systems undergoing phase transitions and enhanced plasticity.

114. COUNCIL ON MATERIALS SCIENCE

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

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.
115. PHYSICAL PROPERTIES OF CERAMIC MATERIALS

W. S. Williams
Phone: (217) 333-3524
$55,000 01-2

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

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

H. Chen
Phone: (217) 333-7636
$75,000 01-3

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

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

W. F. Klemperer
Phone: (217) 333-2995
$100,000 01-3

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

D. A. Payne
Phone: (217) 333-2937
$120,000 01-3


119. MICROSTRUCTURE AND CRYSTALLIZATION IN NOVEL GLASSY SYSTEMS

S. H. Risbud
Phone: (217) 333-2885
$20,000 01-3

Glass synthesis and phase transformations in quasi-binary II-IV-V\textsubscript{2} semiconducting glasses. Electrical, optical and thermomechanical properties of these glasses. Melting, solidification, and glass formation in quasi-binary systems of the Cd-Zn-Ge-As system. Location of N in crystallized glasses. Formation of glass-ceramic composites.

120. MICROWAVE STUDIES OF TUNNELING STATES IN DISORDERED MATERIALS

H. J. Stapleton
Phone: (217) 333-0037
$60,000 01-3

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

121. PROCESSING OF MONODISPERSE CERAMIC POWDERS

C. Zukoski
Phone: (217) 333-7379
$65,000 01-3

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

I. M. Robertson
Phone: (217) 333-6776
$95,000

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

123. LOW-TEMPERATURE STUDIES OF DEFECTS IN SOLIDS

A. C. Anderson
Phone: (217) 333-2866
$95,000

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

124. ELECTRONIC PROPERTIES OF SEMICONDUCTOR SURFACES AND INTERFACES

T.-C. Chiang
Phone: (217) 333-2593
$145,000

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

125. HIGH-FIELD SUPERCONDUCTORS

D. M. Ginsberg
Phone: (217) 333-4356
$50,000

Investigation of high-field superconductors by preparation and detailed characterization of samples and by measurements of critical magnetic field, specific heat, magnetic susceptibility, and neutron diffraction.
126. ULTRASONIC STUDIES OF THE STRUCTURE OF MATTER

A. V. Granato
Phone: (217) 333-2639
$70,000 02-2

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

127. INVESTIGATIONS OF CRYSTAL GROWTH BY MOLECULAR BEAM EPITAXY

H. Morkoc
Phone: (217) 333-0722
$200,000 02-2

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

128. PROPERTIES OF CRYSTALLINE CONDENSED GASES

R. O. Simmons, V. R. Pandharipande
Phone: (217) 333-4170 or (217) 333-8079
$190,000 02-2

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

129. NUCLEAR MAGNETIC RESONANCE IN SOLIDS

C. P. Slichter
Phone: (217) 333-3834
$190,000 02-2

Investigations of layered materials and one dimensional conductors with charge density waves, of Group VIII metal-alumina catalysts, and of spin glasses using nuclear magnetic resonance methods.
130. PHYSICAL PROPERTIES OF ORDERED AND DISORDERED SOLID SOLUTIONS

H. Zabel
Phone: (217) 333-2514
$145,000 02-2

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

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

H. G. Drickamer
Phone: (217) 333-0025
$210,000 03-1

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

132. EXCITON COLLECTION FROM ANTENNA SYSTEMS INTO ACCESSIBLE TRAPS

L. R. Faulkner
Phone: (217) 333-8306
$70,000 03-1

Exciton propagation from absorbing chromophores in polymer films to trapping sites on film surfaces at monolayer coverage. Controlled molecular assemblies of three dimensional reaction systems.
140. STRUCTURE AND PROPERTIES OF TRANSFORMATION INTERFACES

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

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

141. MICROSTRUCTURE, PROPERTIES, ALLOY DESIGN: INORGANIC MATERIALS

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

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

142. SOLID-STATE PHASE TRANSFORMATION MECHANISMS

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

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

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

$1,330,000 01-1

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

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

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

$70,000 01-1

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

145. LOCAL ATOMIC CONFIGURATIONS IN SOLID SOLUTIONS

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

$136,000 01-1

Calculations of long-period superstructures in two dimensions using the ANNNI (axial next-nearest-neighbor Ising) model. Experimental elucidation of atomic rearrangements in periodic antiphase structures in Cu$_3$Pd and Ag$_3$Mg using atomic resolution and high-voltage electron microscopy.
146. COLLABORATIVE RESEARCH BY TRANSMISSION ELECTRON MICROSCOPY

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

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

147. MECHANICAL PROPERTIES OF CERAMICS

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

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

148. ENVIRONMENTALLY AFFECTED CRACK GROWTH IN ENGINEERING MATERIALS

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

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

149. HIGH-TEMPERATURE REACTIONS

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

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

150. STRUCTURE-PROPERTY RELATIONSHIPS IN SEMICONDUCTOR MATERIALS

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

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

151. CHEMICAL PROPERTIES AND PROCESSING OF ADVANCED STRUCTURAL CERAMICS

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

152. STRUCTURE AND ELECTRICAL PROPERTIES OF COMPOSITE MATERIALS

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

$91,000 01-3

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

153. CERAMIC INTERFACES

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

$123,000 01-3

Development of an improved understanding of processes that dictate microstructural changes occurring during both materials fabrication and utilization. Current efforts directed at: development of thermodynamic and kinetic descriptions of the stability of continuous intergranular phases, theoretical assessment of the effects of anisotropic surface and grain-boundary energies on microstructural evolution during sintering, modeling the effects of concurrent grain-boundary migration and tracer self diffusion on calculated apparent grain-boundary diffusivities, and examination of the effects of crystallization and sintering atmosphere on microstructure evolution in compacts of chemically synthesized, amorphous, "monodispersed" TiO₂.

154. FAR-INFRARED SPECTROSCOPY

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

$203,000 02-2

Improved infrared detectors, mixers, and spectrometers are developed and used in experiments in important areas of fundamental and applied physics. Technological developments include a liquid-helium-cooled grating spectrometer for emission spectroscopy, ultrasensitive photoconductive detectors for the 50-200 m wavelength range, improved fabrication techniques for bolometric detectors, development of a microcalorimeter for two-dimensional systems and production of tunable picosecond far-infrared pulses by difference frequency generation. Experiments include measurements of the infrared spectra of molecules adsorbed on metal surfaces, and of one-dimensional charge-density wave conductors, measurements of the heat capacity of adsorbed monolayers, measurements of the infrared photoconductivity of impurities in semiconductors, and a test of the Planck theory of thermal radiation with unprecedented accuracy.
155. EXPERIMENTAL SOLID-STATE PHYSICS AND QUANTUM ELECTRONICS

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

$241,000 02-2

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

156. EXCITATIONS IN SOLIDS

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

$165,000 02-2

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

157. TIME-RESOLVED SPECTROSCOPIES IN SOLIDS

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

$113,000 02-2

The main objective of this project is to utilize picosecond and subpicosecond laser sources to study the ultrafast relaxation processes that occur in laser-induced annealing and melting. Such processes under investigation include electron-phonon interactions, phonon-phonon interactions, and electron-electron interactions. The experiments involve exciting dense electron-hole plasmas in a semiconductor such as GaAs and monitoring the time evolution of the electron and phonon distribution functions by Raman scattering and photoluminescence. Another area of investigation involves the study of nonradiative recombinations of photoexcited carriers at deep traps in semiconductors introduced by doping or electron and neutron irradiation. In addition, nonequilibrium phonons generated during the recombination are monitored by Raman scattering.
158. SUPERCONDUCTIVITY, SUPERCONDUCTING DEVICES, AND 1/F NOISE

J. Clarke
Phone: (415) 642-3069
$241,000 02-2

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

Accelerator and Fusion Research Division - 02 -

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

159. R&D FOR ADVANCED PHOTON SYSTEMS

M. R. Howells, D. T. Attwood, M. Cornacchia, J. N. Marx
Phone: (FTS) 451-4949
$847,000 02-2

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

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

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

161. THEORETICAL STUDIES OF THE ELECTRONIC PROPERTIES OF SOLID SURFACES

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

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

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

$99,000 02-3

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

163. SURFACE, CHEMISORPTION, AND THEORY OF SOLIDS

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

$57,000 02-3

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

164. LOW-TEMPERATURE PROPERTIES OF MATERIALS

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

$100,000 03-1

Understanding the behavior of materials by measurement of their low-temperature properties, particularly specific heats. Much work in the region below 1 K, where the temperature scale is not well established. Research also conducted on methods of temperature measurement. A temperature scale has been developed to 5 mK. Measurements on $^3$He in the Fermiliquid region that have established the correct values of important parameters; measurements on potassium, rubidium, and cesium to 0.06 K to test theoretical predictions of charge-density-wave effects; measurements on CuMn in high magnetic fields that have mapped out the phase boundary of the spin-glass phase; and measurements on a number of heavy-fermion compounds, including two of the three heavy-fermion superconductors, UPt$_3$ and Ube$_{13}$. Future objectives include an extension of the $^3$He measurements to the superfluid phases, studies on spin glasses, and specific-heat measurements at pressures to 20 kbar and in magnetic fields to 9 T on other heavy-fermion compounds.
165. ELECTROCHEMICAL PROCESSES

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

Exploration of novel methods for reducing mass transfer resistance in high rate applications, including in electroforming of metals, and in electrosynthesis. The effects of suspended inert solid particles in flowing electrolytes, on transport rates, and on current distribution are measured over broad ranges of process variables; theoretical models are advanced for the interpretation of mechanisms. Novel approaches are explored for the control of composition and of phase structure in the electrodeposition of alloys. New reaction schemes are evaluated for the efficient electrosynthesis of essential chemicals.

166. HIGH-TEMPERATURE THERMODYNAMICS

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

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

167. CHEMISTRY AND MATERIALS PROBLEMS IN ENERGY PRODUCTION TECHNOLOGIES

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

To characterize the chemical and physical behavior of materials in the high temperature, radiation environment of fission and fusion reactors. The materials of the uranium-based fuels and the zirconium-based cladding materials of light-water nuclear reactors of principal interest. The processes and properties studied include rapid transient vaporization of fuel materials by laser pulsing, high temperature corrosion of zirconium by steam, and the release of volatile fission products from irradiated UO₂. Molecular beam studies of the chemical kinetics of gas-solid reactions, including hydrogen atom reactions with silicon and its compounds and the etching of metals of halogens.
168. ELECTROCHEMICAL PHASE BOUNDARIES

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

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

169. SOLID-STATE AND SURFACE REACTIONS

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

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

170. NUCLEAR MAGNETIC RESONANCE

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

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

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

$47,000 03-3

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

Center for Advanced Materials - 03 -

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

172. CAM ELECTRONIC MATERIALS PROGRAM

Eugene Haller
Phone: (415) 486-5294

$835,000 01-3

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

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

$106,000 01-1

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

174. CAM STRUCTURAL MATERIALS: PROBLEMS IN ALLOY DESIGN

J. W. Morris, Jr.
Phone: (415) 642-3815 or (FTS) 451-6482  
$510,000 01-1

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

175. CAM STRUCTURAL MATERIALS: LIGHT ALLOYS

J. W. Morris, Jr., T. Devine, R. O. Ritchie, G. Thomas
Phone: (415) 642-3815  
$195,000 01-1

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

J. Clarke
Phone: (415) 642-3069

$423,000 02-5

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

177. CAM POLYMERS AND POLYMER COMPOSITES PROGRAM

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

$534,000 03-2

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

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

$792,000 03-3

Synthesis, characterization, and evaluation of surface materials: catalysts, coatings interface compounds and bio-compatible surfaces. Emphases are on microporous solids, metal-oxide interfaces, plasma deposited layers and anchored organometallic molecules to polymer surfaces in the liquid phase. Techniques and instrumentation developments include solid state NMR, scanning tunnel microscopy, electron and laser spectroscopies. The materials under investigation include transition metal carbides, nitrides, alumina silicates, bimetallic (Re-Rt, Su-Pd) systems, oxide-metal (TiO$_2$-M, Al$_2$O$_3$-M, SiO$_2$-M) interfaces and oxide-oxide interfaces (MoO$_x$-Al$_2$O$_3$, V$_2$O$_x$-SiO$_2$). Discovery of new, lower cost catalysts with increased selectivity and resistance to degradation in industrial conditions.
190. RAPID SOLIDIFICATION PROCESSING OF ALLOYS: STRUCTURE, PHASE RELATIONS AND PHASE TRANSFORMATIONS

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

$384,000 01-1

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

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

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

$212,000 01-1

Investigations of microstructures produced in alloy layers created by rapid heating and cooling via electron- or laser-beams and by atomic mixing via ion-beams. Studies of the dependence of crystalline phase and glass formation as a function of binary phase relationships, epitaxial relationships, and resolidification velocity. Studies of the morphology of layers formed from film-on-substrate and bulk alloy starting geometries. Comparisons of laser- and electron-beam processing modes. Analysis using electron microscopy, optical microscopy, X-ray diffraction, Auger and Ion-Beam spectroscopies.
New optical materials suitable for active laser media or transmitting optics in high-power laser systems are prepared and characterized. Properties measured include absorption and emission spectra and cross-sections, lifetimes, nonlinear refractive index, and nonlinear absorption. Ab initio theoretical calculations of energy levels and optical properties of ion-host systems are performed. Physical and chemical mechanisms for optical surface damage are investigated using spatially and temporally resolved photo-emission of electrons and ions, time-of-flight mass spectroscopy surface chemical analysis, and optical emission from laser-excited surfaces.
IRRADIATION-INDUCED METASTABLE STRUCTURES IN METALS AND CERAMICS

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


MECHANICAL PROPERTIES

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

202. STRUCTURAL CERAMICS

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

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

Physics Division - 02 -
J. F. Smith - Phone (FTS) 843-8455 or (505) 667-8455

203. CONDENSED MATTER RESEARCH WITH THE LANSCE FACILITY

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

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

204. MATERIALS UNDER EXTREME CONDITIONS

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

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

J. L. Smith, Z. Fisk, J. D. Thompson
Phone: (505) 667-4476
$96,000

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

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

J. C. Wheatley, G. W. Swift, A. Migliori
Phone: (505) 667-4133
$220,000

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

Materials Chemistry - 03 -

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

207. SURFACE SCIENCE OF CERAMICS

T. N. Taylor
Phone: (505) 667-7712
$58,000

Characterization of majority species on SiC powder surfaces using XPS and LEISS. Correlation of surface chemistry with powder preparation and reactivity. Graphitization of SiC surfaces. Powder surface modification by gas phase reaction, with focus toward improving dispersibility. Comparison of orientationally-averaged powder results with model single crystal experiments. Surface bonding (XPS) and subsurface diffusion (RBS) of selected dopants on SiC, especially the beta-form.
Investigation of synthesis-structure-property relations are studied by iterative application of rigorously controlled synthesis of conducting polymers, detailed physical and chemical characterization of their properties, and detailed theoretical modeling and comparisons with a spectrum of materials and experimental data. Polyacetylene and other analog materials are studied as a class, investigating new synthesis and controlled doping methods.
215. THEORETICAL STUDIES OF METALS AND ALLOYS

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

$685,000 01-1

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

216. X-RAY RESEARCH USING SYNCHROTRON RADIATION

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

$560,000 01-1

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

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

$705,000 01-1

Development and application of analytical electron microscopy (AEM) and atom-probe field-ion microscopy (APFIM) to determine the microstructure and microchemistry of materials. Equilibrium and radiation-induced segregation at grain boundaries and interfaces by APFIM/AEM, correlation of GB structure and segregation. Characterization of ordered and modulated alloys by direct measurement of diffracted electron intensities. Standardless EELS analysis, cross-section measurements for E₀ < 300 kV. Secondary fluorescence in EDS. Lattice site location in alloys by electron channeling microanalysis. APFIM characterization of modulated structures, spinodals, and early stages of phase transformations. GB phases and segregation in structural ceramics, ion-implanted ceramics, crept SiC, precipitates, segregation, and dislocations in Ni₃Al, AEM of supported metal catalysts.

218. RADIATION EFFECTS

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

$1,385,000 01-4

Mechanisms and theory of radiation effects, neutron damage in pure metals, alloys, and ceramics irradiated in ORR, HFIR, EBR-II and FFTF. Effect of alloying additions; impurities and microstructure on dimensional instability and embrittlement; phase stability under irradiation; radiation effects studies using multiple ion beams (heavy and dual light ions); relationship between ion and neutron damage; effect of helium and other gases on microstructure and microcomposition; theory of void swelling and irradiation creep; solute-defect interactions; cascade diffusion theory, Fe, Al, Zr, Ni, and austenitic Fe-Cr-Ni alloys; ferritic alloys; MgO, Al₂O₃, MgAl₂O₄. Ion beam modification of phase relationships, surface-sensitive mechanical properties and microstructure of alloys using multiple simultaneous beams of various species; new materials by ion beam processing.
219. HIGH TEMPERATURE ALLOY DESIGN

Phone: (615) 574-4459
$1,245,000 01-5

Design of ordered intermetallic alloys based on Ni$_3$Al and other aluminides. Study of the effect of alloy stoichiometry on structure and properties of grain boundaries, nature and effects of point defects, and microalloying and grain-boundary segregation. Study of superlattice dislocation structure, solid-solution hardening, mechanistic modeling of anomalous temperature dependence of yield stress, and deformation and fracture behavior of aluminides in controlled environments at elevated temperatures. Study of superplastic behavior, grain-boundary cavitation, and theoretical modeling of creep behavior of Ni$_3$Al alloys. Experimental work on structure and properties of rapidly solidified materials and thermal and physical properties of aluminides. Establishment of correlation between mechanical properties, microstructural features, and defect structures in aluminides.

220. PROCESSING SCIENCE AND MECHANICAL BEHAVIOR OF CERAMICS

P. F. Becher, P. Angelini, S. Baik, A. Bleier
Phone: (615) 574-5157
$945,000 01-5

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

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

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

222. STRUCTURE AND PROPERTIES OF SURFACES AND INTERFACES

Phone: (615) 574-4344

Structure of ion-implanted $\text{Al}_2\text{O}_3$, SiC, and $\text{TiB}_2$ by backscattering-channeling and TEM, hardening, surface fracture toughening and wear of ion-implanted ceramics, structure and properties studied as a function of implantation parameters (temperature, fluence, energy, ion species) and annealing (temperature and environment). Mechanical behavior of thin films and interfaces, stress relaxation and dissipation. Adherence of oxide films. Ion beam mixing and amorphization of multi-layer metallic alloys, mechanical properties.

223. INTERATOMIC INTERACTIONS IN CONDENSED SYSTEMS

Phone: (615) 574-5240

Inelastic neutron scattering studies of phonons, magnons, and single-particle excitations in condensed matter, elastic and inelastic scattering of polarized and unpolarized neutrons by magnetic materials, lattice dynamics of $\text{I}_2$, $\text{Sm}$, $\text{UBe}_13$, and graphite intercalation compounds, magnetic excitations in spin glasses, $\text{USb}$, paramagnetic Ni, Fe, Gd, Sm, and $\text{KMn(Ni)F}_3$, phase transitions in $\text{KTN}$, $\text{Ni}_3\text{Mn}$, Cu(Fe), and random-field systems, nuclear spin ordering in Pr, PrCu$_2$, and Cs$_2\text{NaHoCl}_6$ momentum distributions in $^3\text{He}$ and $^4\text{He}$. New research directions will include more emphasis on materials properties under extreme environments of high pressures, high temperatures or ultralow temperatures.
224. PROPERTIES OF DEFECTS, SUPERCONDUCTORS, AND HYDRIDES

J. W. Cable, H. R. Child, B. D. Gaulin, J. B. Hayter,
H. A. Mook, R. M. Moon, Y. Morii, R. M. Nicklow, H. G. Smith,
S. Spooner, G. D. Wignall

Phone: (615) 574-5233

$656,000 02-1

Elastic, inelastic, and small-angle scattering of neutrons by superconductors, metal hydrides, and defects in single crystals, lattice dynamics of CeD₂, Fe(Cr) alloys, and KCl(CN), magnetic excitations in CeD₂, PrD₂, and K₂(Co)FeF₄, phase transitions in metal alloys, CoCr₂O₄, ZrO₂, heavy fermion superconductors and reentrant superconductors, SANS from ferrofluids, micelles under shear, polymers and polymer blends, metal alloys, and biological systems, kinetics of first-order phase transitions.

225. SUPPORT FOR NEUTRON USERS’ PROGRAM

R. M. Nicklow, J. W. Cable, H. R. Child, B. D. Gaulin,
M. R. Hagen, H. A. Mook, R. M. Moon, H. G. Smith

Phone: (615) 574-5240

$780,000 02-1

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

226. PHYSICAL PROPERTIES OF SUPERCONDUCTORS

S. T. Sekula, D. K. Christen, J. R. Ellis, J. R. Thompson

Phone: (615) 574-6271

$335,000 02-2

Investigations of flux-line-lattice arrays, flux motion, flux-line defect interactions, anisotropy in refractory metal alloys and compounds with Al₅ and B₁ crystal structures, and formation of metastable superconductors by rapid laser quenching, small-angle neutron scattering by flux-line lattices in equilibrium and nonequilibrium configurations, dc magnetization, ac magnetic permeability, critical-current and normal-state electrical transport, ion damage and implantation in foil and thin-film superconductors, low-temperature fast neutron irradiation, pulsed-laser irradiation at low temperatures.
227. SEMICONDUCTOR PHYSICS AND PHOTOPHYSICAL PROCESSES OF SOLAR ENERGY CONVERSION

Phone: (615) 574-6306
$935,000 02-2

Picosecond laser spectroscopy, time-resolved reflectivity, transmissivity, and ellipsometric measurements, time-resolved transient electrical conductivity light-assisted chemical vapor deposition of thin films, modulated layered structures, and superlattices, laser-induced recrystallization of amorphous layers, thermal and laser annealing of lattice damage in Si, Ge, and GaAs, fabrication of high-efficiency solar cells by laser techniques, investigations of thermophotovoltaic systems, effects of point defects, and impurities on electrical and optical properties of single-crystal and polycrystalline Si, electrical, optical (including infrared and luminescence spectroscopy), transmission electron microscopy, X-ray scattering, surface photovoltage, secondary ion mass spectrometry, and Rutherford ion backscattering measurements, dopant concentration profile, deep-level transient spectroscopy, and absolute quantum efficiency measurements.

228. FUNDAMENTAL ASPECTS OF METAL FRACTURE

F. W. Young, S.-J. Chang, C. G. Park
Phone: (615) 574-5501
$360,000 02-2

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

J. B. Bates, F. A. Modine, C. Y. Allison, Y. T. Chu,
N. J. Dudney, G. R. Gruzalski, E. Sonder, J. C. Wang
Phone: (615) 574-6280
$740,000 02-2

Physical and chemical properties of refractory materials, electronic
ceramics, and solid ionic conductors, transition-metal carbides and nitrides
and refractory oxides, physical properties of materials characterized with
regard to composition, defect structures, and phase segregation, studies
involving charge and mass transport with emphasis on varistor materials,
degradation, and high-temperature effects, electrical transport in single-
phase and composite electrolytes, role of adsorbed water on enhanced
cconductivity in AgCl-Al2O3 composites, techniques include optical and
electron spectroscopies and electrical measurements.

230. SOLID-SOLID INTERFACES

Phone: (615) 574-6280
$300,000 02-2

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

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

Preparation and characterization of advanced materials including the growth of single-crystal research specimens and the development of new crystal growth techniques, arc fusion and flux growth of high-temperature materials (Y_2O_3, MgO, CaO, SrO, WC), Czochralski and float zone growth of ternary Fe-Ni-Cr alloys (i.e., stainless steels), rf induction float zone growth of transition-metal carbide single crystals, growth of perovskite-structure oxides (e.g., KTaO_3, CaTiO_3, KTa_1-Nb_0.5O_3), float zone and tri-arc growth of A15 compounds (i.e., V_3Si, Ti_2Pt, V_3Ge), growth of refractory metal single crystals such as Ti, Zr, Ir, Nb, Ta, V, and W by means of the electron beam float zone technique, growth of single crystals of semiconducting oxides (i.e., Ca-doped KTaO_3), flux growth of single crystals of fast ion conductors (beta-alumina and beta"-alumina), growth of single crystals with controlled geometries and isotopically enriched research specimens, characterization studies of single crystals using Rutherford backscattering, ion channeling, EPR, neutron scattering, thermal analysis, and other techniques.

232. SMALL-ANGLE X-RAY SCATTERING

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

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


Phone: (615) 574-5787

$1,164,000 02-3


234. X-RAY DIFFRACTION AND ELECTRON MICROSCOPY

B. C. Larson, J. D. Budai, S. Iida, J. D. Lewis, S. M. Ohr, C. G. Park, S. Pennycook, J. Z. Tischler

Phone: (615) 574-5506

$794,000 02-4

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

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

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

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

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

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

Phone: (615) 574-6291
$895,000 02-5

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

238. SURFACE MODIFICATION AND CHARACTERIZATION FACILITY AND COLLABORATIVE RESEARCH CENTER

Phone: (615) 574-6295
$895,000 02-5

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

Phone: (615) 574-6295 $960,000 02-5

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

240. ION BEAM DEPOSITION

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

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

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

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

Materials Chemistry - 03 -

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

242. CHEMISTRY OF ADVANCED INORGANIC MATERIALS

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

Application of ion implantation and ion beam mixing to the generation and systematic study of surface-modified materials of interest as catalysts, e.g., mixed oxide catalysts on metallic substrates for electrocatalysis of Cl₂ and O₂ evolution; determination of the mechanism of the catalyzed reaction, nature of the catalyst, and its specific mode of operation via electrochemical, Rutherford backscattering, and in situ photoacoustic and photocurrent spectroscopic techniques. SiS-based methodology for the synthesis of high-purity ceramics (alpha-Si₃N₄, SiC, etc.) from relatively impure silicon; synthesis characterization, pyrolysis and photolysis of groups IV-A, V-A, and VI-A transition metal organometallic compounds for the preparation of ceramic powders, fibers, and films; synthesis of transition metal (Ti, Nb, Mo, V, etc.) nitrides and carbonitrides via precursors generated by ammonolytic and metathetical reactions in liquid ammonia; utilization of molten cyanides for the synthesis of BN and TiN ceramics; application of a metal atom reactor to the synthesis of ceramic and ceramic precursor compounds.
243. STRUCTURE AND DYNAMICS OF ADVANCED POLYMERIC MATERIALS

Phone: (FTS) 624-4974 or (615) 574-4974
$1,049,000 03-2

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

244. THERMODYNAMICS AND SENSITIVITY ANALYSES INVOLVING ENERGY-RELATED MATERIALS

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

Determination and modeling of phase equilibria and other thermochemical data important to energy-related ceramic systems. Emphasis on the measurement and application of such data for the actinide oxides used as nuclear fuels, but the methodology is applicable to any oxide solid solution. Current studies involve nonstoichiometric dioxides in the system of elements U, O, and either Y, Ce, Nd, Gd, or Eu. Experimental data are obtained under conditions generally not previously investigated. Adaptations of chemical-mathematical models from the literature are used to represent the chemical thermodynamic interrelationship of temperature, oxygen chemical potential, and nonstoichiometry. These efforts provide a heretofore unavailable, generalized chemical thermodynamic description of the actinide-lanthanide dioxide solutions. Exploratory work involves application of this methodology to structural ceramic systems.
Fundamental laser scattering measurements and theoretical framework for material transport and thermodynamic properties of liquid mixtures at high temperatures and pressures, often in the critical region. Methods development (including optical measurements, dispersion stabilization, and mathematical analysis) for properties measurement of organic mixtures such as those important in critical extraction. Critical region phase equilibrium. Viscosities, diffusivities, and vapor-liquid equilibrium at high pressures and temperatures. Crystallization and growth of monodispersed seed materials, particle size analysis.
A synchrotron radiation beam line installed by the Oak Ridge National Laboratory at the National Synchrotron Light Source at Brookhaven is made available to interested users from university and industrial laboratories. University staff and industrial scientists are invited to join in collaborative research in materials science of importance to DOE programs at a large and unique research facility not available at their home institutions. More than twenty institutions are presently members. The beam line supplies focused X-radiation spanning the energy spectrum from 3 to 40 KeV at energy resolutions of $\delta E/E = 2 \times 10^{-4}$. One Oak Ridge Associated University staff member is stationed at the NSLS to interface with the users and to develop computer programs for data acquisition and analysis. Among the research capabilities available on this beam line are: crystallography on small samples, structure of amorphous materials both liquid and solid, diffuse X-ray scattering from crystalline defects, short-range order and atomic displacements, and X-ray spectroscopy of electron

**256. SHARED RESEARCH EQUIPMENT PROGRAM (SHARE)**

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

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

J. L. Bates, C. F. Windisch
Phone: (509) 375-2579
$330,000 01-1

Mechanisms and kinetics of high-temperature reactions for refractory metal oxides with molten silicates, molten salts, and gases. Dissolution of oxides such as MgAl$_2$O$_4$, Al$_2$O$_3$, MgO, and Y$_3$Al$_5$O$_{12}$ with Ca-Al-silicate containing Mg and Fe in oxidizing, reducing, and sulfur-containing atmospheres. Electrochemical interaction and decomposition of oxides such as ZrO$_2$ in molten salts and silicates. Effects of grain boundary chemistry and structure, crystallographic structure and electrical characteristics on dissolution and electrochemical reactions. Mass transport near reaction interfaces and in grain boundaries from elemental distribution using high resolution, quantitative EDX, electron microprobe, STEM coupled with optical microscopy, TEM, SEM, and AES. Direct in-situ observation of reaction interfaces using laser Raman spectroscopy.

261. FUNDAMENTAL STUDIES OF STRESS CORROSION AND CORROSION FATIGUE MECHANISMS

R. H. Jones, D. R. Baer, M. J. Danielson, M. A. Friesel
Phone: (509) 376-4276
$450,000 01-2

Investigations of the mechanisms controlling intergranular and transgranular stress corrosion and corrosion fatigue cracking of iron, iron-chromium nickel, and nickel-based alloys in gaseous and aqueous environments with and without gamma radiolysis. Relationships between grain boundary chemistry, hydrogen embrittlement, and intergranular stress corrosion cracking investigated with surface analytical tools, electrochemical polarization, straining electrode tests, subcritical crack growth tests, and crack tip and fracture surface analysis. Modeling of the electrochemical conditions at the tip of a growing crack and evaluation of the electrochemical behavior of sulfur and phosphorus in the grain boundaries of nickel. Acoustic emission analysis of stress corrosion cracking processes. Effect of plastic strain and gaseous environments (O$_2$, H$_2$O, and H$_2$O+Cl) on adsorption processes studied with an in-situ Auger electron spectroscopy straining stage.
Mechanistic studies of the interactions of silicate glasses and crystalline ceramics with aqueous environments, by systematic variation of bulk structure, surface properties, and solution chemistry. Structural studies consider the influence of bridging/nonbridging oxygen ratios, extent of polymerization, and redox effects on leachability. Surface electrical properties in solution, sorption phenomena, and the nature of an altered surface layer are included in studies of the effects of surface properties on leaching. Solution chemistry parameters of interest include pH, Eh, ionic strength, saturation with respect to key glass components, and the use of isotopically-labelled water.

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

Solid State Physics - 02 -

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

264. THIN FILM OPTICAL MATERIALS

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

$183,000

Theoretical and experimental study of basic physical properties that control the optical behavior of dielectric materials in thin film form. Measure, model, and understand how the behavior of thin-film optical structures depends on materials properties. Materials studied: elemental semiconductors and their oxides and nitrides. Materials properties studied: composition, stoichiometry, phase structure, strain, and stress. Optical and material characterization techniques include Raman spectroscopy, X-ray diffraction, laser interferometry, total integrated and angular scattering, and resonant cavity reflectometry.
Multidisciplinary studies to relate molecular structure of ceramics to physical properties. Develop models for environment/strained solid interactions used to interpret fatigue effects; Photon Stimulated Desorption (PSD) of in situ fracture surfaces to determine chemical compounds resulting from stress corrosion fracture, model systems to study strain-enhanced chemistry; FTIR studies of adsorbate reactions used to relate strain enhanced chemistry and stress corrosion fracture. Characterize sol-to-gel and gel-to-glass transitions in the silica system using SAXS, HPLC, NMR, and light scattering to determine structures of the pre-gel phase, random colloidal aggregates, and the gel-to-glass conversion; model structure of porous materials using concepts of fractal geometry to predict structure solid material from solution chemistry, and model sintering and absorption characteristics of random porous materials. Study sintering of silicon nitride using oxygen free powders, characterize powder preparation processes.
277. ION IMPLANTATION AND DEFECTS IN MATERIALS

S. T. Picraux, S. M. Myers, K. L. Brower, B. L. Doyle, H. J. Stein,
D. M. Follstaedt, J. A. Knapp, W. R. Wampler, P. S. Peercy, L. E. Pope,
R. B. Diegle, N. R. Sorensen

Phone: (505) 844-7681

$920,000 01-3

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

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

278. ADVANCED GROWTH TECHNIQUES FOR IMPROVED SEMICONDUCTOR STRUCTURES

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

Phone: (505) 844-7681

$186,000 01-3

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

Solid State Physics - 02 -

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

279. SURFACE PHYSICS RESEARCH AND STIMULATED DESORPTION

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

$608,000 02-2

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

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

280. ORGANIC CONDUCTORS AND SUPERCONDUCTORS

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

$327,000 02-2

The fundamental physical properties of the charge transfer organic superconductors and the polymeric organic conductors. Directed toward understanding the detailed band structure, doping, and carrier transport in these materials, especially as they pertain to understanding metal-insulator transitions, superconductivity, and the role of disorder in determining transport properties. Unique and specialized instrumental capabilities including high frequency magnetic resonance, conductivity, photoconductivity, thermal conductivity, heat capacity, magnetotransport, de Haas van Alphen, thermopower and tunneling. Experiments at temperatures as low as 0.05 K, magnetic fields up to 120 kOe and hydrostatic pressure to 10 kbar in various combinations. An active in-house synthesis program in collaboration with J. Williams at Argonne National Laboratory supports the measurement programs and develops new materials. The in-house synthesis of novel charge transfer organic superconductors and the chemical and electrochemical growth of very high purity polymeric organic conductors.
281. CHEMICAL VAPOR DEPOSITION AND SURFACE PHOTOKINETIC RESEARCH

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

Studies of important vapor-phase reactions and nucleation processes during CVD deposition under conditions used to fabricate photovoltaic cells, corrosion-resistant coatings, and semiconductor devices. Measurements of major and minor species densities, gas temperatures, fluid flows, and gas-phase particulate distributions using laser Raman and Mie scattering and laser induced fluorescence. Test of our predictive model, which includes chemical and fluid dynamics. Study and development of laser CVD, laser photochemical deposition and etching, and laser-based fabrication of small-dimension structures. Application of our laser-based measurement capabilities to the study of vapor phase reactions of these laser processing techniques and application of surface measurement techniques to study the product materials. Fundamental study of the interactions of photons and molecules near and on surfaces. Auger, Sims, and laser-based measurements of surfaces in situ to deposition and etching. Development of model for combined laser, admolecule, and surface dynamics.
Studies of the initial stages of deposition phenomena relevant to combustion and material processing environments. Utilize in situ, nonintrusive optical diagnostics to probe reactions at fluid/solid and solid/solid interfaces. Linear and nonlinear spectroscopies applied to dynamics of deposit layer evolution. Applications including combustion-flow deposits, high-temperature corrosion, materials joining, ceramic surface chemistry, and surface segregation.

Investigations of the behavior of hydrogen, tritium and helium in metals involving joint theoretical and experimental research. Experimental techniques include mechanical property measurements, electron microscopy, positron annihilation, and small angle neutron scattering, applied to tritiated metals and also metals implanted with helium below the damage threshold. A new theoretical method (Embedded Atom Method) developed to calculate the cohesive energy of metals and alloys with chemically active impurities which is being used to investigate the atomistic processes of fracture, dislocation motion, and chemistry at surfaces and grain boundaries. Investigate equilibrium structure of alloys, such as Ni 3 Al, both in the bulk and at interfaces including the effects of adsorbates and alloying additions.
292. THIN SURFACE LAYER REACTIONS

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

$240,000 02-2

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

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

$100,600

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

296. SEMICONDUCTOR THEORY

A. Zunger
Phone: (303) 231-1172

$105,400

This project focuses on the application of first-principles band structure and total energy calculation techniques to the study of the electronic and structural properties of semiconductors, including the prediction of chemical trends and properties of new materials of potential photovoltaic interest, and the prediction of structural parameters and relative stabilities of these systems. The prototypical systems studied include: (i) disordered semiconductor alloys (e.g. Si_x Ge_{1-x}, Ga_y In_{1-x}P), (ii) novel ordered phases of alloys (e.g. SiGe, GaInP, CdMnTe), (iii) The Nowotny-Juza ternary semiconductors AlB_{1-C}V (e.g. LiZnAs), (iv) ternary chalcoprytes Al_{III-C}VI_{2} (e.g. CuInSe_2) and (v) ternary pnictide AlIB_{IV-C}V_2 (e.g. ZnSiP_2). The theoretical tools used include: the total energy non-local pseudo-potential method and (b) the all-electron Mixed Basis Potential Variation band structure method. This work also includes the study of deep defects in semiconductors: e.g. chemical trends for 3d impurity levels in different host crystals (including alloys), prediction of hitherto unobserved impurity levels and excited states and understanding of the lattice distortions induced in the host, and the clarification of their likely impact on device characteristics. The theoretical technique used for the impurity studies is the Quasi-Band Crystal Field Green's function method.
Support of materials research utilizing synchrotron radiation, as well as operations and development of the Stanford Synchrotron Radiation Laboratory (SSRL). Development and utilization of new methods for determining atomic arrangements in amorphous materials, static and time-resolved studies of highly perfect semiconductor crystals using X-ray topography, photoemission studies of semiconductor interfaces (e.g., heterojunctions and Schottky barriers), metal surfaces (especially catalytic reactions on surfaces) and development of techniques such as surface EXAFS, photoelectron diffraction, photon stimulated desorption and interface studies using core level spectroscopy.
SECTION B

Grant Research
(Primarily Universities)

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

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

$104,250 02-2

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

302. ARTIFICIALLY LAYERED SUPERCONDUCTORS

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

$91,396 02-2

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

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

Response of ceramic materials to multiaxial stress states. Consideration of: (a) surface condition, (b) test geometry, and (c) environment. Control of each of the above variables so individual effects can be studied, specimen preparation to insure that the flaw population is isotropic and material directionality is eliminated. Relationship of stress-state effects to stress-intensity factor, effects of tensile and shear stresses parallel to an artificial crack and effects of stress ratios on strength in ceramic specimens containing natural flaws to evaluate statistical (Weibull) descriptions of strength. Material characterization, fractography, three-dimensional linear elastic finite element analysis of test-specimen geometries and stress-intensity factors. High-temperature biaxial tension tests of ceramic specimens containing controlled artificial flaws. Materials of interest: Al₂O₃, Si₃N₄, glass-ceramics, and partially stabilized ZrO₂.

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

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

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

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

$130,000 (16 Months) 02-2

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

306. TWO-DIMENSIONAL COLLOIDAL SYSTEMS

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

$51,000 02-2

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

307. SYNTHESIS AND PROPERTIES OF NOVEL, ELECTROACTIVE ORGANOMETALLIC POLYMERS

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

$80,955 03-2

Synthesis of organometallic polymers based on transition metal complexation of rigidly held aromatic five and six membered rings. The aromatic ring will be held in a framework such that electron or hole conduction should occur through overlap of the pi-orbitals on contiguous facing aromatic rings. The C₅-based polymers will be derived from paracyclophenes and the C₅ polymers from cyclopentadienylnaphthalene.

BRIGHAM YOUNG UNIVERSITY  
Provo, UT 84602

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

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

$50,979 01-2

Studies of intergranular creep cavitation in alloy 304 stainless steel as a function of a) grain boundary misorientation angle, b) grain boundary surface orientation, and c) multiaxial stress state. SEM and TEM diffraction characterizations of boundary structure and cavitation damage. Processing effects on grain boundary structure distribution and damage susceptibility.
This research involves experimental and modeling efforts addressing the deformation and fracture of various steels. Emphasis is placed on developing a detailed correlation between mechanical behavior and microstructural features in structural alloys, specifically regarding the limits of uniform ductility, necking strain and fracture toughness, shear localization at notch tips, propagation of surface cracks under fully plastic conditions, and hydrogen-enhanced void growth in steels deformed under different strain states.

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

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

$98,768 01-2

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

312. SURFACES AND THIN FILMS STUDIED BY PICOSECOND ULTRASONICS

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

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

$216,000 02-2

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

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


314. STUDIES OF ALLOY STRUCTURE AND PROPERTIES

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

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

315. MELTING IN ADSORBED FILMS

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

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

A. K. Mukherjee  
Dept. of Mechanical Engineering  
Phone: (916) 752-1776, 0580  
$31,300 01-2

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

317. CHEMICAL DECOMPOSITION OF CERAMICS UNDER IRRADIATION

D. G. Howitt  
Dept. of Mechanical Engineering  
Phone: (916) 752-0580  
$71,000 (6 months) 01-4

Investigation of electron and ion irradiation induced ionization, displacement damage, diffusion, and stimulated desorption by means of in situ electron microscopy and mass spectroscopy. Study of ion mixing effects under ion irradiation. Finite difference solutions to a two-dimensional diffusion equation for the irradiation and desorption process. Materials: Na-Al2O3, Na borosilicate glass, TiC.

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

Z. A. Munir  
Dept. of Mechanical Engineering  
Phone: (916) 752-0559  
$100,291 01-5

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

320. SURFACE EXCITATIONS AND THEIR INTERACTION WITH LOW ENERGY ELECTRONS

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

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

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

C. N. J. Wagner  
Dept. of Materials Science and Engineering  
Phone: (213) 825-6265  
$102,934 01-4

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

322. RESEARCH ON THE THERMOPHYSICAL PROPERTIES OF MATERIALS

G. A. Williams  
Dept. of Physics  
Phone: (213) 825-8536  
$180,000 02-5

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

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

$336,378 02-2

An investigation of superconductivity and magnetism and the interaction of these phenomena in binary and ternary transition metal, rare earth and actinide compounds. Emphasis on RRh$_4$B$_4$, R being a rare earth, where superconductivity and long range magnetic order are known to exist, and on heavy fermion systems. A search for superconducting and unusual semiconducting compounds of cerium and uranium. Changes in superconducting and magnetic properties of compounds prepared by nonequilibrium techniques such as shock compression.

324. ION MIXING AND SURFACE MODIFICATION IN METAL SEMICONDUCTOR SYSTEMS

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

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

$200,845 (15 months) 02-4

Investigation of the physical mechanisms responsible for ion-mixing effects in metal-semiconductor systems. Generalize and predict ion-induced reactions, correlations between ion-induced reactions and those induced by conventional thermal annealing. Physical mechanisms and conditions necessary for the formation of a specific reaction product determined. Different metal-silicon systems investigated. Sample configurations include metal layer on silicon bilayers, multi-layers, and alloy thin film structures. Primary experimental tools: ion implantation, thermal annealing, Rutherford backscattering, Auger electron spectroscopy, X-ray diffraction, and transmission electron spectroscopy. A collaborative program between the University of California, San Diego, and Cornell University including interaction with Oak Ridge National Laboratory.
B-12

UNIVERSITY OF CALIFORNIA/SANTA BARBARA
Santa Barbara, CA 93106

325. CONDENSED MATTER RESEARCH USING THE UCSB FREE ELECTRON LASER

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

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

$115,500 02-2

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

326. RESEARCH ON PATTERN FORMATION IN SYSTEMS FAR FROM EQUILIBRIUM

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

$107,975 02-3

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

327. NUMERICAL SIMULATION OF QUANTUM MANY-BODY SYSTEMS

D. J. Scalapino
Physics Dept.
Phone: (805) 961-2871

J. R. Schrieffer
Physics Dept.
Phone: (805) 961-2280

R. L. Sugar
Physics Dept.
Phone: (805) 961-3469

$113,384 02-3

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

CARNEGIE MELLON UNIVERSITY
Pittsburgh, PA 15213

328. THE EFFECT OF STRESS ON PRECIPITATE MORPHOLOGY

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

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

$107,651 01-1

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

I. M. Bernstein  
Dept. of Metallurgical Engineering and Materials Science  
Phone: (412) 268-2700

A. W. Thompson  
Dept. of Metallurgical Engineering and Materials Science  
Phone: (412) 268-2711

G. W. Warren  
Dept. of Metallurgical Engineering and Materials Science  
Phone: (412) 268-2700

$114,314 01-2

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

CASE WESTERN RESERVE UNIVERSITY  
Cleveland, OH  44106

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

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

$149,110 01-2

Ostwald ripening in ZrO$_2$ toughened Al$_2$O$_3$. Plastic deformation in two phase "single crystal" Ca partially-stabilized ZrO$_2$, and in 100 percent tetragonal ZrO$_2$ polycrystals. Stress-induced transformation in Y-TZP and ZTA. The focus of these studies is the nature and extent of the transformation zone associated with propagating cracks and the critical factors involved in processing strong and tough polycrystalline tetragonal ZrO$_2$. Correlation of TEM analysis with mechanical properties.
331. RESEARCH IN THE THEORY OF CONDENSED MATTER AND ELEMENTARY PARTICLES

L. P. Kadanoff  
The James Franck Institute  
Phone: (312) 962-7189

Y. Nambu  
The James Franck Institute  
Phone: (312) 962-7286

D. Friedan  
Dept. of Physics  
Phone: (312) 962-7119

S. Shenker  
Dept. of Physics  
Phone: (312) 962-7187

$185,000 02-3

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

332. SURFACE CHEMISTRY OF ELECTROCATALYSIS

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

$81,000 03-2

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

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

Investigation of the mechanism of formation and decay of electrets in nonpolar inorganic polycrystalline and amorphous dielectrics. Experimental characterization of electret formation with sample temperature, polarization field, and cooling rate, and of electret decay in the open and closed circuit condition. Extension of Swann-Gubkin theory by considering the nonpolar part of electret polarization through the displacement of ions to account for the production of nonpolar electrets. Materials of interest include CaTiO₃, SrTiO₃, BaO₄, TiO₂, BiTiO₃, (SrBi)TiO₃, chalcogenide glasses and elemental Se. X-ray diffraction. Thermally stimulated discharge current analysis.

334. PHYSICAL METALLURGY OF FERROUS ALLOY WELD METAL

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

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

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

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

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

$42,977 02-2

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

COLORADO STATE UNIVERSITY
Fort Collins, CO 80525

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

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

$72,423 02-3

Theoretical calculation of the properties of molecular solids and fluids over broad ranges of high temperatures and pressures. Properties of interest are as follows. Solids: equilibrium structures and orientations, lattice vibrational and librational mode frequencies, intramolecular vibron frequencies, sound velocities, equations of state, compressibilities, and structural and orientational phase transitions. Fluid phase: equations of state, vibron frequencies, the melting transition, specific heats, compressibilities, second virial coefficients, viscosities and other transport properties, and the nature of orientational and magnetic correlations. Techniques used include multi-dimensional optimization strategies, self-consistent lattice dynamics, constant pressure and constant volume Monte Carlo (i.e., variable metric) computation, mean field and classical perturbation methods. Systems studied include N$_2$, O$_2$, CO, CO$_2$, F$_2$, N$_2$O, benzine, nitromethane, HCl, HBr, and H$_2$. Attention is given to connections to combustion and detonation phenomena, and to synthesis of new materials.
337. STUDIES OF MELTING, CRYSTALLIZATION, AND COMMENSURATE-INCOMMENSURATE TRANSITIONS IN TWO DIMENSIONS

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

Preparation and study of systems of synthetic colloidal microspheres that exhibit the primary phenomena of physical interest in lower dimensional systems. Use of e-beam lithography and film deposition for construction of substrate particle-traps in extended or local patterns, to provide potential fields acting on the colloidal particles. Quasi-elastic light scattering microscopy and various other optical techniques applied to study colloidal particles in suspension films monolayers, and bilipid membranes. Melting, crystallization, solid-solid transitions, fractal scale invariant coagulation, response of monolayer crystals to equivalent of ultra high pressures, experimental and computer simulation of collapse of particle distributions on quenching electrostatic interparticle forces, critical diffusion rates in thin binary liquid films.

COLUMBIA UNIVERSITY  
New York, NY 10027

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

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

Ion transport processes in perovskite-structured oxides which can be converted into high-temperature protonic conductors by treatment in water vapor. Determination of the manner in which protons enter the host crystal and the appropriate kinetic parameters (e.g., activation energies and association energies) that determine the rate of migration. Monitoring of proton content by observation of intensity of infrared absorption due to the OH$^-$ stretching mode. Investigative techniques include ionic conductivity (complex impedance as a function of frequency), diffusion measurements (including H <-> D interchange), dielectric and anelastic relaxation, electrolyte cell measurements, EPR, NMR, and HADES type computer simulations. Materials of investigation: single crystal KTaO$_3$, sintered polycrystal SrCeO$_3$, SrTiO$_3$, and other perovskite oxides.
339. THE FATIGUE BEHAVIOR OF FERRITIC STEELS AT ELEVATED TEMPERATURES

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

$55,508 01-1

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

340. ELECTRODE STUDIES IN MOLTEN SALTS

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

$11,143 01-3


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

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

$91,600 02-2

Investigation of four aspects of the interaction of single or multiple optical fields with a rare earth ion and its host matrix to elucidate the non-linear optical properties and energy transfer in the system. These aspects are: the optical gain and loss in Ce³⁺:LiYF₄; the non-radiative relaxation processes and the ion-lattice interactions associated with the 5d->4f transition; photoconductivity due to excited states of rare earth ions in crystals and glasses; and phase conjugate wave generation and laser-induced grating studies at near ultraviolet wavelengths.
342. THE MIGRATION OF GRAIN BOUNDARIES IN CERAMICS WITH PARTICULAR REFERENCE TO THE SINTERING PROCESS

C. B. Carter
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Phone: (607) 255-4797

Study of the effect of geometry and composition of interfaces on interfacial mobility in ionic-covalent solids. Concerns include (1) misorientation between grains and boundary plane orientation, (2) geometry of interfacial dislocations and steps, (3) interfacial chemistry including local segregation and nonstoichiometry, and (4) interfacial pinning by pores or crystalline or amorphous pockets or films of a second phase. Materials of investigation include \( \text{Al}_2\text{O}_3, \text{MgO}, \text{NiO}, \text{Mg-Al spinel}, \text{Si}, \text{Ge}, \text{Si}_3\text{N}_4, \) and \( \text{SiC}. \) Studies on both powder compacts and bicrystals involve visible light microscopy, electron microprobe analysis, and strong- and weak-beam, lattice fringe, X-ray energy dispersive, and electron energy loss TEM analysis.

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

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

N. W. Ashcroft
Dept. of Physics
Phone: (607) 255-3309

Investigation of grain boundary structure of BCC metals, ceramics, and intermetallic compounds using transmission electron microscopy and electron diffraction, and X-ray diffraction techniques, study of the influence of segregation on the structure of grain boundaries in Fe-base alloys, MgO + Fe and Ni\textsubscript{3}Al, determination of grain boundary region in order to obtain structural information, study theoretically the structure of crystalline defects including grain boundaries, and the interatomic potentials needed to calculate their structure.
344. AN INVESTIGATION OF MECHANICAL BEHAVIOR OF POLYCRYSTALLINE SOLIDS

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

$192,400. 01-2

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

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

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

$121,361 01-2

Basic research will include both experimental and modeling tasks with goals to predict failure times of continuous-fiber reinforced polymer composites under load and relate the mean lifetime to fiber and matrix properties. Theoretical effort using probabilistic statistics to derive a distribution of composite strengths; will incorporate distributions of individual fiber strengths and flaws in the composite, local load sharing rules around initial flaws, and viscoelastic properties of the matrix. Experimental effort will involve creep-rupture testing of "microcomposites" to evaluate the models.
Role of inhomogeneities (both second phases and agglomerates) and shear strain in the densification of powder. Elucidation of the mechanisms of densification and flaw generation during high-temperature processing of TiO$_2$ and TiO$_2$-Al$_2$O$_3$ powder compacts with inhomogeneous microstructures. Influence of agglomerates, non-uniform packing, and second phase constituents on the densification process. Measurement of sintering pressure. Free sintering, hot-pressing, and sintering under superimposed hydrostatic pressure experiments on TiO$_2$ on Al$_2$O$_3$ (model material for dry processing) and Si$_3$N$_4$ (with a liquid phase additive for wet processing). Colloidal processing of powder.
Study the correlation between the electronic properties, atomic structure, and local chemistry of defects in GaAs, GaAs-based ternaries and at the interface between GaAs, GaAs-based ternaries and Si. The main objectives of the proposed research:

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

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

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

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

(5) Investigate the origin of CL contrast of Si-GaAs and its connection to the spatial variation of deep states, using a combination of EBIC, CL, TEM, and spatially resolved PL.
INTERNATIONAL CONFERENCE ON THE STRUCTURE, PROPERTIES, AND PROCESSING RELATIONSHIPS OF INTERNAL INTERFACES

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

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

$5,000 01-3

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

STRONGLY INTERACTING FERMION SYSTEMS: EMPHASIS ON HEAVY FERMIONS

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

$120,000 02-3

Theory of heavy fermion behavior in lanthanide and actinide compounds, and more generally of systems with f and/or d electrons that are strongly interacting or correlated. Aims at understanding the occurrence or absence of heavy fermions in such systems, the nature of the low temperature coherent state and the transition to a Kondo-like state at higher temperatures, and of course, at an account of the unusual magnetic and superconducting properties of heavy fermion. Extension to magnetically concentrated systems of approaches known from experience with magnetically dilute alloys, including renormalization study of two-impurity models. Close interaction with ongoing experimental programs at DOE laboratories and elsewhere. Exploration and development of new theoretical and computational methods, for example utilizing functional-integral formulations, discretizing on a lattice in space and temperature, renormalization transformations, and Monte Carlo technique with a Langevin equation for non-perturbative calculation of properties.
350. THE ROLE OF GRAIN BOUNDARIES ON THE STRENGTH, DUCTILITY, AND TOUGHNESS OF L12 INTERMEDIATE COMPOUNDS

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

Examine dislocation pileup/grain boundary accommodation model in more detail, carry out systematic in situ TEM deformation studies on Ni-rich, stoichiometric and Ni-lean Ni₃Al both with (0.35at%) and without boron; investigate grain boundary sliding in Ni₃Al by systematic experiments on the effects of grain size on high-temperature deformation (800-1200K) of Ni₃Al with (0.35at%) and without boron; investigate grain size effects on the strength and ductility of Ni₃Si by systematic experiments on the effects of grain size on the mechanical properties and resultant deformation structure; improve the toughness of Ni₃Al through grain shape control, i.e., generate equiaxed fine grain structure with simultaneous increase of aspect ratio, comparative tests (fibrous vs. equiaxed microstructures) performed at RT using Charpy impact technique. Subsequent fracture toughness measurements using standard ASTM procedures.

351. DURABILITY OF SHORT FIBER COMPOSITE MATERIALS

T.-W. Chou
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Phone: (302) 451-2904

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

352. NEUTRON STUDIES OF LIQUID AND SOLID HELIUM

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

$ 67,340 02-1

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

UNIVERSITY OF DENVER
Denver, CO 80208

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

P. K. Predecki
Dept. of Engineering
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$69,911 01-2

Investigation of residual stresses and strains in ceramic fiber/ceramic matrix composites by X-ray diffraction to obtain the near surface stresses and neutron diffraction to obtain the bulk microstresses in each crystalline phase. Diffraction measurements as a function of temperature on well-characterized specimens--initially from other laboratories--in which either the thermal expansion of the matrix or the fiber surface treatment is systematically varied. Materials investigated include Al$_2$O$_3$ fibers in silicate glasses and glass ceramics, and SiC whiskers in Al$_2$O$_3$. Noyan-Cohen analysis accounting for 3-dimensional nature of stresses and including, where possible, separation of macrostress and microstress components in each phase. Results correlated with mechanical properties and thermal expansion via existing models for composite behavior. The objective is to provide a test for such models and to see if the techniques used are useful for predicting the strength, toughness, and thermal expansion of these materials.
354. DETECTING AND MONITORING CRACK INITIATION AND GROWTH IN AUSTENITIC AND FERRITIC STEELS

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

$69,520 01-5

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

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

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S. A. Safron
Dept. of Chemistry
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$125,060 02-2

Construction of a He atom-surface scattering instrument and the study of the dynamics of crystalline surfaces by low energy He-atom scattering. Extraction from surface phonon data of information on the interactions between surface species and hence on their physical and chemical properties. Surface phonon dispersion curves obtained by time-of-flight methods from inelastic single atom-surface encounters. Corrugation of and energy levels in the He-surface potential, obtained from elastic specular and diffractive scattering. Information on relaxation phenomena obtained from measurements of phonon lifetimes. Studies envisaged include: (110) surfaces of Au, Pt, and Ir, which reconstruct as a function of temperature. Surfaces of active metals (Ni, Cu), both clean and with physisorbed or chemisorbed layers. Surface phonon anomalies in high Tc superconductors. Surfaces of layered dichalcogenide compounds (e.g., TaSe₂, NbSe₂), which exhibit a variety of transitions with decreasing temperature -- including charge density wave formation.
356. THE COUPLING OF THERMOCHEMISTRY AND PHASE DIAGRAMS FOR GROUP III-V SEMICONDUCTOR SYSTEMS

T. J. Anderson
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Phone: (904) 392-2591

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

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

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

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

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

J. J. Hren  
Dept. of Materials Science and Engineering  
Phone: (904) 392-6985  
$80,025 01-3

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

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

M. D. Sacks  
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J. W. Williams  
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Phone: (904) 392-6698  
C. D. Batich  
Dept. of Materials Science and Engineering  
Phone: (904) 392-6630  
$114,863 01-3

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

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

$78,000 02-2

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

361. STUDIES OF HEAVY FERMION SYSTEMS

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

$185,000 02-2

Experimental investigations of "heavy fermion" systems such as UBe$_{13}$ and UPt$_3$ (irradiated), mainly through low temperature calorimetry, but also with electrical resistivity and magnetic susceptibility techniques. The goals of this research: examination of the interactions between f-electron sites and comparison with theoretical models proposed to explain the highly correlated high effective mass observed in heavy fermion systems; observation of the interplay between superconductivity, magnetism, and non-ordered behavior.

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

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G. B. Butler
Dept. of Chemistry
Phone: (904) 392-2012

$98,008 03-1

Synthesis of graft copolymers based on polysaccharides and plysaccharide derivatives and synthesis of model polymers including water-soluble block copolymers, star polymers, and cyclic polymers. Grafting by redox initiation, thermal decomposition, or nucleophilic displacement. Characterization by IR, NMR, size exclusion chromatography, viscometry, and osmometry. Studies of structure-rheology relationships.
GEORGIA TECH RESEARCH CORPORATION
Atlanta, GA 30332-3368

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

A. Saxena
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$104,179 01-2

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

364. CRYSTALLINE METAL-SEMICONDUCTOR SUPERLATTICES

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

$125,000 02-2

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

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

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

$181,000 02-3

Theoretical investigation of the fundamental processes that determine the structure, transformations, growth, electronic properties and reactivity of materials and material surfaces. Analytical methods and molecular dynamics simulation development and application to phase transformations, solidification, laser annealing, defect formation, transport phenomena and chemical reactivity with emphasis on systems relevant to energy technologies.
366. LOCAL MANY-BODY EFFECTS IN THE OPTICAL RESPONSE OF NARROW BAND SOLIDS

A. Zangwill  
Dept. of Physics  
Phone: (404) 894-7333

D. Liberman  
Lawrence Livermore National Laboratory  
Phone: (415) 423-0505

$53,782 02-3

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

367. A CARBANION APPROACH TO POLYACETYLENE

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

$73,000 03-1

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

W. Paul
Div. of Applied Sciences
Phone: (617) 495-2853
$130,000 02-2

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

369. FUNDAMENTAL PROPERTIES OF SPIN-POLARIZED QUANTUM SYSTEMS

I. F. Silvera
Dept. of Physics
Phone: (617) 495-9075, 2872
$229,000 02-2

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

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

M. McNallan
Dept. of Civil Engineering, Mechanics and Metallurgy
Phone: (312) 996-2436
$38,495 01-3

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

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

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

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

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

Investigation of the new iron:rare-earth:metalloid alloys with high potential for permanent magnetic applications including Fe$_{77}$R$_{15}$M$_8$ and Fe$_{82}$R$_{12}$M$_6$ where R is primarily a rare-earth and M is a metalloid such as B, C, and Si. Main emphasis on preparation techniques, correlation of magnetic properties of sputtering films with sputtering parameters, exploration of dependence of the magnetic properties on the electronic factors and atomic spacings in Fe-Nd-B alloys, and a detailed study of the relationship of microstructure, secondary phases and defects on the magnetization reversal and hysteresis. Work in collaboration with the University of Nebraska.
UNIVERSITY OF KENTUCKY
Lexington, KY 40506

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

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

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

374. STRUCTURAL AND SURFACE CHARACTERIZATION OF DISPERSED METAL CATALYSTS

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

Detailed structural and compositional characterization of metallic catalyst particles dispersed on porous oxide supports. Techniques such as analytical electron microscopy, X-ray diffraction, and energy dispersive and ion scattering spectrosopies will be used to examine the dispersed metal catalysts at various stages in their preparation to elucidate the role of strong and weak metal-support interactions on particle morphological development and particle thermal stability.
LEHIGH UNIVERSITY
Bethlehem, PA 18015

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

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

$71,847

Application of analytical, high resolution, controlled atmosphere, and high voltage electron microscopies to understand mechanisms of catalyst promotion and poisoning, and to locate particular species with respect to crystallographic site and surface topographic specifics in the support phase. Systems of interest include the Cu/ZnO and Cs/MoS$_2$ catalyst systems, Cs promoters, and Tl poisons. Near edge fine structure electron energy loss spectroscopy.

376. ANALYTICAL ELECTRON MICROSCOPY STUDIES OF PRECIPITATION IN CERAMIC SYSTEMS

M. R. Notis
Materials Research Center
Phone: (215) 861-4225

D. B. Williams
Materials Research Center
Phone: (215) 861-4220

M. P. Harmer
Materials Research Center
Phone: (215) 861-4220

$130,000

Study of precipitation phenomena by means of analytical and high resolution electron microscopy, laser Raman spectroscopy and X-ray diffraction. Phase transformations resulting in transformation toughening in ZrO$_2$ containing ceramics. Precipitate dissolution kinetics and transient second phase phenomena in the Y$_2$O$_3$-La$_2$O$_3$ system. Precipitate coarsening kinetics in NiO and CoO, and precipitation processes in mullite and glass ceramic materials.
LEHIGH UNIVERSITY (continued)

377. THE EFFECT OF POINT DEFECTS ON STRUCTURAL PHASE TRANSITIONS

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

$87,000 01-1

Study of the coupling of the Li defect to the B\text{1g} soft phonon mode in MnF\text{2}:Li and MgF\text{2}:Li by Raman scattering and infrared absorption. Measurement of ultrasonic attenuation as a function of temperature from 4.2\text{K} so as to estimate the coupling of the Li defect relaxation to the B\text{1g} soft phonon mode. Raman frequency shift, acoustic and dielectric measurements in KMnF\text{3}:Li at temperatures spanning the cubic-tetragonal phase transition so as to identify the Li defect. Neutron scattering measurements in the constant Q-mode and as a function of temperature in Q range centered on the transition temperature with the triple axis spectrometer at the BNL-HFBR. Similar ultrasonic, Raman, and neutron scattering studies on KTa(Nb,Sc)O\text{3} and PbZr(Sc,Mg)O\text{3}.

378. INVESTIGATIONS OF CREEP CAVITATION IN TYPE 304 STAINLESS STEEL

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

$74,060 01-2

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

379. CORROSION FATIGUE OF SMALL CRACKS: MECHANICS AND CHEMISTRY

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

$151,180 01-2

Experimental and theoretical study of corrosion fatigue of NiCrMoV and 304 stainless steels in aqueous solutions, kinetics of growth of small fatigue cracks as a function of frequency, solution chemistry, temperature and crack length, electrochemical reaction kinetics as a function of temperature in the same environment, relating fatigue crack growth response to the electrochemical reaction kinetics, modeling of electrochemical conditions near the crack tip and of the electrochemical and micromechanics aspects of small-crack growth.
380. GRAIN BOUNDARY DIFFUSION IN ORIENTED Ni$_3$Al BICRYSTALS CONTAINING BORON

Y-T. Chou
Division of Metallurgy and Materials Engineering
Phone: (215) 861-3020
$83,530 01-3

Measurement of grain boundary diffusion coefficients in B doped and undoped [001]/[100] tilt bicrystals of Ni$_3$Al. Preparation of such bicrystals.

381. GASES ON METAL SURFACES: ADSORPTION AND PHASE TRANSITIONS

T. L. Einstein
Dept. of Physics
Phone: (301) 454-3419
R. E. Glover III
Dept. of Physics
Phone: (301) 454-3417
R. L. Park
Dept. of Physics
Phone: (301) 454-4127
$ 39,100 02-2

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

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

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

$348,440

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

383. BASIC RESEARCH IN CRYSTALLINE AND NONCRYSTALLINE CERAMIC SYSTEMS

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

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

$398,938

Electrical and optical behavior of Al₂O₃ and MgO including vacuum ultraviolet spectroscopy characterization of band gaps. Float zone laser crystal growth and zone refining in Al₂O₃. Grain boundary migration in high purity powder and bicrystals of Al₂O₃. Kinetic studies include oxygen diffusion measurements in MgO by gas exchange and SIMS, reaction processes and microstructure development in low-temperature sub-solidus systems, rapid quenching effects in a eutectic Ca-Mg-silicate liquid phase and the Fe-Cu two phase system, suppression of insulator charging in SEM and SIMS measurements, grain boundary diffusion in SrTiO₃, and Bi and O grain boundary diffusion in ZnO. Defect structures, defect interaction, grain boundary and surface studies including point defects in SiC, B, and C distribution in doped SiC, grain boundary microchemistry and slow crack growth in SiC, influence of microstructure and grain boundary segregation on electrical properties of polycrystalline ZnO, grain boundary segregation in polycrystalline Al₂O₃, segregation at special grain boundaries in MgO, influence at grain boundary composition on grain boundary diffusion, structure of a migrating low angle tilt grain boundary in SrTiO₃, and role of grain boundary segregation on high temperature deformation in SiC and Al₂O₃. Sintering studies include atom transport, processing and sintering of SiC, grain boundary mobility in alkali halides, test of the applicability of Herring's scaling law, the effect of MgO on sintering of Al₂O₃, and orientation effects on the grain boundary migration of high purity Al₂O₃.
384. MECHANISMS OF TRANSFORMATION TOUGHENING

G. B. Olson
Dept. of Materials Science and Engineering
Phone: (617) 253-6901

I.-W. Chen
Dept. of Materials Science and Engineering
Phone: (617) 253-6901

D. M. Parks
Dept. of Materials Science and Engineering
Phone: (617) 253-6901

$188,745 01-2

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

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

G. Kalonji
Dept. of Materials Science and Engineering
Phone: (617) 253-6863

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

$115,498 01-3

Rapid solidification studies of the systems $\text{Al}_2\text{O}_3$-$\text{ZrO}_2$, $\text{Al}_2\text{O}_3$-$\text{MgO}$, $\text{Y}_2\text{O}_3$-$\text{ZrO}_2$, selected ternary compositions from the previous binary systems, Ba ferrite, and Ni-Zn ferrite. Sample preparation by means of a 1500 watt CO$_2$ laser to melt feed rods of the desired composition, melt spinning, a 1000 watt CO$_2$ laser to perform surface melting and regrowth experiments at controlled solid-liquid interface velocities, and ultrasonic atomization. Sample characterization by means of STEM, XRD, EXAFS, IR and Raman spectroscopy, vibrating sample magnetometry and B-H hysteresis loops and magnetic permeability for soft ferrites.
386. STRUCTURAL DISORDER AND TRANSPORT IN TERNARY OXIDES WITH PYROCHLRE STRUCTURE

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

$100,000  01-3

Relationship of electrical and optical properties to the defect structure in ternary compounds with a pyrochlore structure. Characterization of AC complex impedance of rare earth titanate and zirconate pyrochlores under conditions of controlled composition, temperature, and chemical environment. Optical absorption and emission measurements to monitor the degree of disorder. Preparation of single and polycrystalline samples of known cation-anion ratio by pyrolysis of metal-citrate complex precursors. Complementary sample characterization by thermogravimetric analysis, X-ray diffraction, and Raman spectroscopy. Specific pyrochlores to be investigated are \( \text{Gd}_2\text{Zr}_2\text{O}_7 \) and solid solutions in the \( \text{Gd}_2\text{Zr}_2\text{O}_7-\text{Dy}_2\text{Zr}_2\text{O}_7 \) and \( \text{Gd}_2\text{Zr}_2\text{O}_7-\text{Gd}_2\text{Ti}_2\text{O}_7 \) systems.

387. MECHANISMS OF THE OXIDATION OF METALS AND ALLOYS

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

$182,000  01-3

This research project is investigating the mechanisms of oxidation and oxidation/sulfidation of metals at elevated temperatures. Emphasis will be placed on behavior of alloys that form protective refractory oxide scales such as \( \text{Cr}_2\text{O}_3 \) and \( \text{Al}_2\text{O}_3 \) during oxidation and on factors controlling scale degradation in gas mixture having a high sulfur to oxygen activity. In addition, the influence of very fine-grained microstructures (rapidly solidified materials) of the substrate on mechanisms of oxide formation and breakdown in gas mixtures will be examined.
B-42

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

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

L. W. Hobbs
Dept. of Materials Science and Engineering
Phone: (617) 253-6835
$154,270
01-4

Fundamental research to characterize the irradiation stability and radiation damage microstructures of crystalline ceramic solids with application to nuclear energy production and disposal of high-level nuclear waste. The principal mode of investigation is transmission electron microscopy. Materials to be examined include BeO, MgO, Al<sub>2</sub>O<sub>3</sub>, CaF<sub>2</sub>, PuO<sub>2</sub>, ZrO<sub>2</sub>, SiC, Si<sub>3</sub>N<sub>4</sub>, Li<sub>2</sub>O, LiAlO<sub>2</sub>, LiAl<sub>5</sub>O<sub>8</sub>, Li<sub>2</sub>ZrO<sub>3</sub>, Ca(Zr,Pu)Ti<sub>2</sub>O<sub>7</sub>, titanate pyrochlores, SiO, GeO, ZrSiO<sub>4</sub>. Neutron, ion and electron irradiation damage will be studied, including the effects of massive recoil nuclei and fission fragments.

389. PHYSICS AND CHEMISTRY OF PACKING FINE CERAMIC POWDERS

H. K. Bowen
Dept. of Materials Science and Engineering
Phone: (617) 253-6892
$125,015 (17 months)
01-5


390. LOW TEMPERATURE AND NEUTRON PHYSICS STUDIES

C. G. Shull
Dept. of Physics
Phone: (617) 253-4812
$156,607
02-1

MASSACHUSETTS Institute OF TECHNOLOGY (continued)

391. SUBMICRON LAYERS OF Nb-Al

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

Basic studies of the properties of layered structures as prototypical systems of low temperature reacted niobium-aluminum. Bilayers and multilayers of Nb and Al employed to investigate the effects on the physical properties of structure, composition and content of oxygen and other additives. Study of proximity effects and mechanisms for high critical current in thin layers. Methods of achieving optimum atomic order in these structures will be sought. Research on the applicability of these studies to a wider class of other promising high critical current, field and temperature Nb$_3$X compounds.

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

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

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

The A15 compound V$_3$Ga is the best known superconducting material for the fabrication of practical high field magnets, restricted however, to critical magnetic fields of about 25T. It is believed that this restriction is due to Pauli paramagnetism in the presence of weak spin-orbit (SO) scattering by the low-Z elemental components, and that it can be eased by increasing the SO scattering rate -- which is believed to scale with the fourth power of the atomic number Z. Two approaches to increasing the SO scattering rate: inclusion of high-Z impurities placed randomly but with minimal introduction of lattice disorder, and inclusion of thin closely spaced layers of high-Z materials. Samples prepared by electron beam evaporation and characterized by superconducting properties, resistivity, and spin-polarized tunneling measurements. Aim to test existing theoretical concepts, to advance understanding of high field superconductors and of many-body effects in normal transition metal systems, to develop improved magnetic solenoids.
MIAMI UNIVERSITY
Oxford, OH 45056

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

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

$55,000 02-2

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

MICHIGAN STATE UNIVERSITY
East Lansing, MI 48824

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

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

$70,981 01-2

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

L. A. Heldt
Dept. of Metallurgical Eng.
Phone: (906) 487-2630
M. B. Hintz
Dept. of Metallurgical Eng.
Phone: (906) 487-2630
$93,000  01-2

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

396. THEORY OF DEFECTS IN NON-METALLIC SOLIDS

A. B. Kunz
Dept. of Physics and Institute of Condensed Matter Studies
Phone: (906) 487-2277
$99,000 (16 months)  02-3

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

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

Study the role and mechanism of nucleating agents on the crystallization of the Si$_2$N$_2$O containing boundary phases which are formed during the processing of Si$_3$N$_4$ (containing Y$_2$O$_3$ and Al$_2$O$_3$) and SIALON ceramics including SIALON-Cordierite. Microstructure and phase identification in sintered and hot pressed specimens. X-ray diffraction, scanning transmission electron microscopy, electron energy loss spectroscopy, fractography analysis.

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

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

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

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

P. K. Bhattacharya
Dept. of Electrical Engineering and Computer Science
Phone: (313) 763-6678

A. Brown
Dept. of Electrical Engineering and Computer Science
Phone: (313) 763-3350

R. Gibala
Dept. of Materials and Metallurgical Engineering
Phone: (313) 763-4970

$125,060 01-3

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

400. GROWTH AND DYNAMICS OF SCALE INVARIANT MATTER

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

R. Savit
Dept. of Physics

$155,000 02-3

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

R. A. Oriani  
Dept. of Chemical Engineering and Materials Science  
Phone: (612) 373-4864

D. A. Shores  
Dept. of Chemical Engineering and Materials Science  
Phone: (612) 373-4183

W. H. Smyrl  
Dept. of Chemical Engineering and Materials Science  
Phone: (612) 373-2763

$840,579 01-1

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

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

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

$83,827 01-2

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

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

$104,705 (15 months) 02-2

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

UNIVERSITY OF MISSOURI/COLUMBIA
Columbia, MO 65211

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

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

$55,947 02-2

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

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

$80,557 02-2

A variety of condensed matter experiments using the 46.5 keV Mossbauer transition in tungsten-183 produced at the Missouri University Research Reactor, which is a thousand times more intense than conventional Mossbauer sources. Quasi-elastic scattering in a liquid metal study of self-diffusion as a function of temperature; Elastic-inelastic separation of the diffracted radiation in zinc to study large anomalous anharmonic contributions to the scattering; A determination of the charge density wave satellites in TaS$_2$ near the commensurate-incommensurate first order phase transition. An improved measurement of the asymmetry parameter of the 46.5 keV transition. Experiments to separate the elastic and inelastic scattering at Bragg reflections for measurement of the quasi-elastic linewidths near critical points. Signal to noise for these experiments enhanced through the use of a specially developed microscopic conversion electron (MICE) detector: additional isotopes will be tried. In collaboration with J. G. Mullen at Purdue.

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

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

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

$76,472 01-1

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

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

$119,288 01-3

Interrelationships between electrical conductivity, oxidation-reduction kinetics, defect structure, and composition for n- and p-type binary and ternary transition metal oxides. Focus on the influence of electric fields and oxygen activity gradients on oxide-electrode stability, oxygen transport through oxides, and dopant energy levels in oxides. Experiments include specimen preparation, thermogravimetric characterization, optical microscopy, X-ray diffraction, TEM, electrical conductivity, EPR, thermally stimulated current, optical absorption, and oxygen diffusion.

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

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

$ 51,560 02-2

Investigation of the new iron:rare-earth:metalloid alloys with high potential for permanent magnetic applications including Fe$_{77}$R$_{15}$M$_{5}$ and Fe$_{82}$R$_{12}$M$_{6}$ where R is primarily a rare-earth and M is a metalloid such as B, C, and Si. Main emphasis on preparation techniques, correlation of magnetic properties of sputtering films with sputtering parameters, exploration of dependence of the magnetic properties on the electronic factors and atomic spacings in Fe-Nd-B alloys, and a detailed study of the relationship of microstructure, secondary phases and defects on the magnetization reversal and hysteresis. Work in collaboration with Kansas State University.
409. ENERGY TRANSFER BY TRIPLET EXCITON MIGRATION IN POLYMERIC SYSTEMS

R. D. Burkhart  
Dept. of Chemistry  
Phone: (702) 784-6041  
$90,000 03-1

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

410. RADIATION EFFECTS AND ANNEALING KINETICS IN Crystalline Complex Nb-Ta-Ti oxides, phosphates, and silicates

R. C. Ewing  
Dept. of Geology  
Phone: (415) 277-4163  
$75,902 01-1

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

C. L. Beckel
Dept. of Physics
Phone: (505) 277-2449

V. M. Kenkre
Dept. of Physics
Phone: (505) 277-2616

D. Emin
Dept. of Physics
Phone: (505) 277-8602

$176,000 (2 years) 02-3

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

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

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

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

$105,657 01-1

Preparation of thin-film surface coatings by glow discharge and reactive sputtering of disordered alloys of carbon, silicon, and hydrogen ($C_{x}Si_{y}H_z$) with carbon as the primary constituent. Characterization using photoemission, EXAFS, optical spectroscopy (visible and IR) and measurements of density and hardness. Photoemission and carbon K-edge absorption studies using synchrotron radiation at the BNL NSLS.
413. DYNAMICS OF FLUID SURFACES AND THE CRYSTAL-MELT INTERFACE

H. Z. Cummins  
Dept. of Physics  
Phone: (212) 690-6921  
$112,704 02-2

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

414. MAGNETIC PROPERTIES OF DOPED SEMICONDUCTORS

M. Sarachik  
Dept. of Physics  
Phone: (212) 690-8206  
$100,000 02-2

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

415. CONDUCTION AND PROPAGATION IN DISORDERED SYSTEMS

M. Lax  
Dept. of Physics  
Phone: (212) 690-6864, (201) 582-6527  
$113,153 02-3

Theoretical research concerned, in part, with hopping conductivity in multidimensional systems, including quasi-one-dimensional organic chains such as polyacetylene, and even DNA. Work on the production, propagation, screening and isotope scattering of terahertz phonons in GaAs. Application of multiple scattering techniques to scattering from random, wavy surfaces. Emphasis on transport in small systems whose size can be comparable to the mean free path.
416. DIRECT SYNTHESIS AND OPTIMIZATION OF Fe-BASED, RARE-EARTH, TRANSITION METAL PERMANENT MAGNET SYSTEMS

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

Prepare and characterize polycomponent metal films of Nd$_2$Fe$_{14}$B, and related R$_2$Fe$_{14}$B systems, (Sm + Ti)Fe$_5$, Sm(Ti,Fe)$_2$ and Sm$_2$(Co,Fe,Zr)$_17$ under a variety of conditions by RF sputtering. Films made with and without a composition gradient along the length of the substrates. Selectively thermalized sputtering employed to yield highly textured and metastable structures to aid in the direct growth of crystallographically orientated samples. X-ray diffraction, X-ray fluorescence analysis and electron microprobe will be employed to determine crystal structure and composition variations. High field magnetization and electron energy loss spectroscopy measurements on films with varying crystallographic texturing-selected magneto-optical measurements will be carried out.

417. MIXED VALENT BEHAVIOR IN ACTINIDES AND RELATIONSHIP TO CERIUM

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

Theoretical research on the manybody aspects of materials containing the early actinide elements and cerium. Principal subject areas: the direct relationships between the magnetic properties, conduction electron-spin scattering effects in transport properties, and the single particle excitation spectrum (as seen in photoemission and Bremsstrahlung Isochromat spectroscopies). Basic theoretical model: a lattice of magnetic ions (the Anderson Lattice) in which the magnetic f-electrons can be delocalized by both the direct f-f overlap and the hybridization with the valence band. Also a study of electron phonon-mediated couplings and other possible exotic coupling mechanisms in the heavy fermion superconductors CeCu$_2$Si$_2$, UBe$_3$, and UPt$_3$. 
STATE UNIVERSITY OF NEW YORK/BUFFALO
BUFFALO, NY 14214

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

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

$400,000 02-2

Development of facilities at the National Synchrotron Light Source for X-ray diffraction, X-ray absorption spectroscopy, and other X-ray scattering techniques by a participating research team composed of professors from many of the State University of New York campuses, Alfred University, Roswell Park Memorial Institutions, Cortland State College, Geneseo, the University of New Orleans and Allied Corporation. The research interests are: structure of materials, electronic structure of materials, surface physics, compositional analysis, and time-dependent biological phenomena.

STATE UNIVERSITY OF NEW YORK/STONY BROOK
Stony Brook, NY 11794

419. INTERFACE PROPERTIES AND CRYSTAL-GROWTH MECHANISMS

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

$69,861 01-1

Use of computer simulation methods to examine synergistic effects of roughening and surface melting in crystal-vapor systems; mechanism of impurity incorporation in rapidly growing crystals; anisotropy of growth velocity with different crystal faces in crystal-melt systems; incidence of melt regions forming in grain boundaries at high temperatures; rough-smooth transitions observed in MBE grown crystal-vapor systems; influence of directional bonding (e.g., in network formers like Si) on interface width, growth, velocity, impurity trapping, and roughening temperature.
Implementation of facilities and research for the Synchrotron Topography Project beamline X-19C at the National Synchrotron Light Source at Brookhaven National Laboratory under the auspices of a National Consortium headed by the SUNY Stony Brook group. The consortium is continuing work on a wide range of problems where the special properties of synchrotron radiation are particularly suited including: studies of the factors controlling elastic-plastic crack propagation, real-time slip initiation observations, quality assessment of crystal growth, mechanical integrity of thin film-substrate interfaces, thermal decomposition mechanisms for inorganic single crystals, in situ measurements of the film stresses accompanying film deposition for refractory metal silicides on silicon, detailed studies of the interaction of acoustic waves with microstructural constituents, morphology of pressure quenched CdS and X-ray topography and microradiography aimed at understanding high temperature deformation mechanisms of steels.

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

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

422. KINETICS OF PHASE SEPARATION IN POLYMER SOLUTIONS

B. Chu
Dept. of Chemistry
Phone: (516) 246-7792
$85,000 03-1

Kinetics of phase separation in polymer solutions and blends. Structure of phase separated droplets. Size, shape, and distribution of micro domains measured using light and X-ray scattering, excimer fluorescence, and optical microscopy. Phase separation kinetics measured using time-resolved, small-angle X-ray scattering at the National Synchrotron Light Source. Studies of polymer-solvent systems, such as polystyrene-methylacetate, and polymer-polymer blends, such as polystyrene blended with polyvinyl methyl ether, polyisoprene, or polyorthochlorostyrene.

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

J. L. Whitten
Dept. of Chemistry
Phone: (516) 246-6068
$100,000 03-3

Theoretical study of the structure and energetics of molecules adsorbed on solid surfaces and dissociative chemiadsorption with emphasis on transition metal substrates. Systems studied are titanium, copper, nickel and copper/nickel substrates, and H₂, H, CO, C and coabsorbed H and C adsorbates. Emphasis is on the energetics of adsorption as a function of surface site and composition to determine the reactivity of adsorbed species. Theory focuses on an accurate, ab initio treatment of the localized and delocalized interactions that occur in the case of adsorption on metals with active d electrons.
424. PHOTOEMISSION STUDIES OF F-ELECTRON SYSTEMS: MANY BODY EFFECTS

S. J. Williamson
Dept. of Physics
Phone: (212) 598-2867
$100,000 02-2

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

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

V. S. Avva
Dept. of Mechanical Engineering
Phone: (919) 379-7620
J. Sankar
Dept. of Mechanical Engineering
Phone: (919) 379-7620
$67,340 01-5

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

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

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

$86,903 (15 months) 02-2

Measurements of low-frequency vibrational properties of disordered solids in the far infrared region (5 cm$^{-1}$ to 150 cm$^{-1}$) as a function of temperature using laser techniques. Materials studied: various forms of quartz and fused silica, alumina and magnesia. Other materials of interest: BeO, BN, and Si$_3$N$_4$. Effects on dielectric properties due to the presence and concentration of impurities and sintering acids, and to microstructural properties, investigated in selected materials. Experimental data compared with existing theoretical models.

427. MICROSTRUCTURAL EFFECTS IN SOLID PARTICLE EROSION

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

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

$91,153 01-5

Correlation of erosion rates in multiphase systems with constituent phase properties and distribution. Systems under investigation: Al-Si alloys, WC-Co cerments, SiC-reinforced alumina and alumina-stainless steel composites, and sintered alumina. Systematic measurement of erosion rates as a function of operational variables (particle size, velocity, angle-of-incidence) and microstructural variables (volume fraction, phase size and distribution, alloy content). SEM observations on steady-state erosion surfaces and single impact events. Constitutive and averaging laws for erosion rates to be developed from experimental results and modeling/computer simulation.
428. DEVELOPMENT OF AN X-RAY BEAM LINE AT THE NSLS FOR PRT STUDIES IN MATERIAL SCIENCE USING X-RAY ABSORPTION SPECTROSCOPY

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

$315,000 02-2

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

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

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

$105,000 03-1

Theoretical studies of superconducting and conducting, organic charge transfer salts. Tight-binding band electronic structure calculations on bis(ethylenedithio)tetrathiafulvalene (ET) salts using extended Huckel method. SCF-MO calculations on neutral and charged ET. Calculation of crystal packing energies, stabilities of different crystal phases, and magnitudes of electron-phonon coupling constants of various ET salts.
A theoretical program for investigating the behavior of positrons in imperfect metallic systems and at metallic surfaces. Appropriate generalizations of the current multiple scattering theory techniques undertaken to develop framework capable of describing a wide range of phenomena on a realistic basis. Systems to be investigated: metal and alloy surfaces, metallic glasses, vacancies and vacancy-impurity complexes, and substitutional alloys. Characteristic features of the annihilation process between the positrons and the electrons delineated. A close collaboration with relevant experimental groups planned.

Comprehensive investigation of Sn fibers deposited in UHV on single crystal CdTe substrate including the study of quantum size effect using high-resolution electron energy loss spectroscopy and optical absorption, determination of relationship between thermal degradation and interfacial diffusion in heterojunctions, determination of film growth characteristics using a site-specific xenon probe technique, and determination of structural and transformation characteristics using surface XRD at the NSLS and electron reflectivity techniques.
Interdisciplinary study of the first row transition metal monoxides, combining measurements of defect structure and electrical properties with quantum theoretical calculations. These oxides represent a "model" series which, while sharing the average structure of NaCl, exhibit a wide range of stoichiometries, defect structures, and conduction mechanisms. Electrical measurements and conduction mechanism analysis will be extended to MnO and NiO. Valence in the series will be studied via X-ray (synchrotron) and/or pulsed neutron scattering. The self consistent field local density theory will be used to calculate the electronic structure associated with isolated vacancies and defect clusters. An energy band code based on the Linearized Muffin Tin Scheme will be used to calculate band structures, Fermi surfaces, and transport properties to correlate with the experimental studies. Extension of theory will be made to more complex oxides, e.g., Fe$_3$O$_4$, CoAl$_2$O$_4$, and FeAl$_2$O$_4$. 
433. NUCLEAR MAGNETIC RESONANCE CHARACTERIZATION OF POROUS STRUCTURES: CERAMICS AND SANDSTONES

W. P. Halperin
Physics and Astronomy Department
Phone: (312) 491-3686
$89,629 01-1

Application of nuclear magnetic resonance measurements (spin-lattice relaxation and variable length scale diffusion) using a variable length scale pulsed field gradient method (VLS/PFG) to filler fluid nuclei intruded into the pore space of porous materials to give specific information concerning void space microstructure. Experiments with model materials including leached borosilicate (vycor) glasses and packings of monodisperse glass spheres. Investigations of fractal sandstones to define fractal dimension, minimum and maximum fractal length scales, and random-walk dimension for dynamics confined to a fractal. Non-fractal sandstones also investigated to obtain structural parameters and clarify the distinction between dynamics in fractal and non-fractal geometries. Investigation of pore structure evolution in the early and the intermediate stages of sintering of alumina by NMR methods giving direct information on the pore size distribution, throat size, maximum extent of the pore distribution and the distribution of pore surface-to-volume ratios. Evolution of these parameters studied as a function of heating rate and initial compact conditions. Experiments to help to refine sintering models and define relevant processing parameters for attainment of high density.

434. USE OF ANOMALOUS SMALL ANGLE X-RAY SCATTERING TO INVESTIGATE MICROSTRUCTURAL FEATURES IN COMPLEX ALLOYS

J. R. Weertman
Dept. of Materials Science and Engineering
Phone: (312) 491-5353
$80,848 01-2

Investigation of the use of anomalous small angle X-ray scattering (SAXS) to break down the scattering from a complex alloy into the components arising from each of the different scattering species, thereby making it possible to use the SAXS data to obtain quantitative information about the size and number density of each species. Synchrotron radiation will be used to provide X-rays which can be tuned to the absorption edge of elements in the alloy. Anomalous SAXS will be used to characterize the various scattering species in systems of interest and to study the changes in these scatterers produced by exposure to high temperature and deformation. The first system to be studied will be the ferritic stainless steel, modified Fe9Cr1Mo, which has already been examined by small angle neutron scattering. The value of anomalous SAXS as a method of NDE will be investigated.
435. DEFECT STRUCTURE OF SEMICONDUCTING AND INSULATING OXIDES

B. W. Wessels
Dept. of Materials Science and Engineering
Phone: (312) 491-3219
$77,466 01-3

Use of space charge spectroscopy techniques to explore the deep level electronic defect structure and its role in charge transport for several semiconducting and semi-insulating oxide compounds. Single crystalline oxide layers prepared by organometallic chemical vapor deposition. Defect phenomena investigated include mechanisms of deep level defect formation, thermal stability of native point defects, and the electrical and optical characterization of deep level defects in as-grown undoped and doped material. Deep level defects formed by high energy electron and proton irradiation. Isochronal annealing. Experimental point defect characterization includes temperature dependent conductivity and photoluminescence measurements. Specific systems to be examined include ZnO, TiO$_2$, and SrTiO$_3$.

436. STRUCTURAL AND FAST ION TRANSPORT PROPERTIES OF GLASSY AND AMORPHOUS MATERIALS

D. H. Whitmore
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Phone: (312) 491-3533
P. Georgopoulos
Dept. of Materials Science and Engineering
Phone: (312) 491-3243
$116,000 01-3

Detailed structural and ionic transport studies of fast ion conducting glasses including mixed valence, proton conducting and selenide based glasses and amorphous polyphosphazene polymer complexes. Investigation parameters include temperature, glass composition, and conditions of glass synthesis. Computer simulations of ionic transport in glassy electrolytes. Differential anomalous X-ray scattering, EXAFS, Raman and infrared spectroscopies, complex impedance analysis (of conductivity data) and pulsed field gradient NMR (to obtain ionic diffusivities). Mixed valence glasses synthesized by doping glass network formers with appropriate amounts of transition metal compounds investigated for the chemical diffusion coefficient, solid-state redox reactions accompanying the insertion of electroactive alkali ion species into the mixed valence glass and the electronic transference number as a function of glass composition and temperature.
437. LOCAL DENSITY THEORY OF HEATS OF FORMATION AND SHORT-RANGE-ORDER PARAMETERS IN SUBSTITUTIONALLY DISORDERED ALLOYS

A. J. Freeman  
Dept. of Physics and Astronomy  
Phone: (312) 491-3343, 3644  
A. Gonis  
Dept. of Physics and Astronomy  
Phone: (312) 491-3644  
$76,956 02-3

Determination of thermodynamic properties and, ultimately, phase diagrams of ordered and substitutionally disordered alloys from all-electron calculations that utilize fully relativistic energy band programs and that take into account lattice structure and statistical fluctuations. Particular emphasis is given to heats of formation, to short-range order parameters, and to polyatomic interaction energies. Recently developed methods based on local density theory, on embedded cluster generalizations of the coherent potential approximation, and on a generalized perturbation method are used to obtain the density of states and total energies. Multi-site potentials obtained are to be used, e.g., in cluster variation method computations to construct alloy phase diagrams for transition metals (and, perhaps, actinides).

438. STUDIES OF THE SHEAR RESPONSE AND STRUCTURE OF MONOMOLECULAR FILMS ON THE SURFACE OF WATER

P. Dutta  
Dept. of Physics and Astronomy  
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J. B. Ketterson  
Dept. of Physics and Astronomy  
Phone: (312) 492-5468  
$91,302 03-3

Study of the mechanical properties of organic monolayers on the surface of water (Langmuir films). The microscopic structure of such films and of multilayers formed on repeatedly dipped substrates (Langmuir-Blodgett films) studied using X-rays and ellipsometry. Studies of the mechanical properties directed toward the shear response, an important but previously neglected structural property. A diffraction technique involving external reflection at the monolayer surface used to determine structure. Finally the loss of certain symmetry elements of surface phases studied by observing the rotation of plane polarized light incident normal to the surface. A search for this effect within the so-called liquid expanded-liquid-condensed region, which may be a liquid crystal phase.
UNIVERSITY OF NOTRE DAME
Notre Dame, IN 46556

439. MICROSTRUCTURAL EFFECTS IN ABRASIVE WEAR

T. H. Kosel
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Phone: (219) 239-5642

Assessment of mechanisms controlling abrasive wear in multiphase Fe- and Co-base alloys, influence of second phase particle toughness, size and volume fraction, changes in near-surface microstructure during abrasion, influence of abrasive size, hardness, angularity and loading conditions, in situ SEM scratch test simulations of fixed-abrasive abrasion mechanisms.

OHIO STATE UNIVERSITY
Columbus, OH 43210

440. INFLUENCE OF NITROGEN ON THE SENSITIZATION, CORROSION, MECHANICAL AND MICROSTRUCTURAL PROPERTIES OF AUSTENITIC STAINLESS STEELS

W. A. T. Clark
Dept. of Metallurgical Engineering
Phone: (614) 422-2538
B. E. Wilde
Dept. of Metallurgical Engineering
Phone: (614) 422-7889

Evaluation of corrosion and stress corrosion cracking of austenitic stainless steel with various carbon and nitrogen contents. TEM characterization of grain boundary structure as well as carbide and nitride morphologies, compositions, and distributions. Measurement of electrochemical parameters in static and flowing aqueous solutions containing chloride and sulphate ions.

441. FUNDAMENTAL STUDIES OF HIGH TEMPERATURE CORROSION REACTIONS

R. A. Rapp
Dept. of Metallurgical Engineering
Phone: (614) 422-6178

In situ SEM study of oxidation of metals, Fe, Ni, Cu and Cr, and binary alloys of these metals, effect of H₂ on oxide morphology, influence of surface treatment on oxidation of Cr, pore development at metal-scale interface, oxide morphologies, e.g., pits and ledges in Fe₂O₃ and whiskers in NiO.
OHIO STATE UNIVERSITY (continued)

442. GENERATION OF MICROPOROSITY IN STEEL WELDS AND ITS ROLE IN HYDROGEN ATTACK

P. G. Shewmon
Dept. of Metallurgical Engineering
Phone: (614) 422-5864

Investigation of mechanisms controlling hydrogen attack in bainitic steels, with emphasis on evaluating degradation in weldments made by various processes—gas tungsten and submerged arc welding as well as electroslag welding, characterization of microporosity with electron microscopy (both TEM and SEM) and dilatometry, respectively, to indicate the microstructural features where attack initiates and the overall kinetics of attack, assessment of role of matrix creep and of susceptibility of fusion vs. heat affected zone to attack.

443. INVESTIGATIONS OF ULTRASONIC WAVE INTERACTIONS AT BOUNDARIES SEPARATING ANISOTROPIC MATERIALS

L. Adler
Dept. of Welding Engineering
Phone: (614) 422-1974

This is a basic research program on non-destructive characterization of polycrystalline anisotropic materials. Specific activities will include modeling and measurement of ultrasonic wave propagation in bicrystals of Ni and austenitic stainless steel as well as fabrication of specimens and development of techniques.

444. MOLECULAR FERROMAGNETISM

A. J. Epstein
Dept. of Physics
Phone: (614) 422-1133

Study of magnetism in molecular ferromagnets and origins of the ferromagnetic exchange. Synthesis of \([\text{M(C}_5\text{H}_5\text{)}_2]^+\) and \([\text{M(C}_6\text{R}_6)]^+\) (M=Cr, Fe, Ru, and Ni) salts of planar radical anions 7,7,8,8-tetracyano-p-quinodimethane (TCNQ), tetracyanoethene (TCNE), and 2,3-dichloro-5,6-dicyanobenzoquinone (DDQ). Measurements of magnetism as a function of field, temperature, and pressure and comparison of results with models of one-dimensional ferro- and ferri-magnetism. Mossbauer spectroscopy to measure internal magnetic fields, spectroscopic measurements of charge transfer bands, and inelastic neutron scattering measurements of magnetic structure.
445. PERTURBED ANGULAR CORRELATIONS IN ZR-CONTAINING CERAMICS

J. A. Gardner
Dept. of Physics
Phone: (503) 754-4631

$58,000 01-1

Perturbed angular correlation (PAC) spectroscopy of nuclear gamma rays to investigate Zr-containing ceramics. PAC characterization of free energies and transformation mechanisms in ZrO$_2$ based materials. Measurement of ZrO$_2$ equilibrium phase boundaries and their dependence on purity and stabilizing elements. Analysis of relaxation models and diffusion mechanisms in ZrO$_2$-Y$_2$O$_3$ alloys, short range order and order-disorder reactions, and high-temperature time-dependent effects in various stabilized zirconias. Design and construction of a pressure cell for operation at 200 MPa and 2000°C.

446. SURFACE AND INTERFACE ELECTRONIC STRUCTURE

S. D. Kevan
Dept. of Physics
Phone: (503) 686-4742

$143,500 02-2

An experimental investigation of the electronic structure of surfaces and interfaces including studies of angle-resolved photoemission at the National Synchrotron Light Source. Emphasis on high resolution studies of novel surface phenomena such as phase transitions, small perturbations of the ground state electronic structure by defects and impurities, and initial stages of epitaxial interface formation between metals and semiconductors.

447. MONITORING INTERFACIAL DYNAMICS BY PULSED LASER TECHNIQUES

G. L. Richmond
Dept. of Chemistry
Phone: (503) 686-4635

$70,125 03-2

Studies of interfacial structure and dynamics using second harmonic generation (SHG) and hyper-Raman scattering. Development of SHG for monitoring electrochemical reactions on a nanosecond and picosecond time-scales, correlation of surface structure and electron-transfer reactivity, thin film nucleation and growth, and analyses of the structure and reactive role of surface defects.
448. PHYSICAL CHEMISTRY OF PORTLAND-CEMENT HYDRATE, RADIOACTIVE-WASTE HOSTS

M. W. Grutzeck
Materials Research Laboratory
Phone: (814) 863-2779

$61,977 01-1

Physical and crystal chemistry of three portland-cement hydrates: calcium silicate hydrates, calcium aluminum hydrates, and calcium alumino silicate hydrates. Phase-equilibrium relationships governing the hydration of portland cement, both with and without radioactive waste. Fixation of iodine by calcium aluminate hydrates and the feasibility of using Stratling's compound and its associated hydrates as host phases for cesium and strontium fixation. Identification of phases best suited for hosting selected radioactive-waste ions, and synthesis and crystallographic characterization of such phases. Solubility/leachability study of synthesized host phases both individually and encapsulated in a suitable cementitious matrix.

449. VIBRATIONAL AND OPTICAL STUDIES OF AMORPHOUS METALS

J. S. Lannin
Dept. of Physics
Phone: (814) 865-9231

$87,792 01-1

Research aimed at developing the method of interference enhanced Raman scattering (IERS) to study the structure, bonding, and stability of amorphous metal alloys. The basis of the IERS technique is to fabricate thin film trilayer structures of the materials to be studied which include a dielectric layer and a reflecting layer to produce a minimum in the reflectance and thus reduce the background light when measuring the Raman scattered light. Focus is initially on metalloid alloys and will subsequently be extended to amorphous metals in general. Complementary inelastic neutron scattering measurements are also employed for structure, bonding, and short-range order determinations.
450. SPECTROSCOPIC INVESTIGATIONS OF GLASS STRUCTURE

W. B. White
Materials Research Laboratory
Phone: (814) 865-1152

$43,480 (9 months) 01-1

Glasses containing transition metal ions are studied utilizing Raman, infrared, optical absorption, and luminescence spectroscopy. Specific investigations include (i) the local environment of alkali ions in silicate glasses by far infrared spectroscopy, (ii) processes of phase separations as related to heat treatment by high-temperature Raman spectroscopy, (iii) the relationship of Raman spectra to thermodynamic quantities in silicate glasses, (iv) formation of transition metal complexes in glass, and (v) clustering and nucleation of transition meals in high magnesium content glasses.

451. THE MECHANICAL BEHAVIOR OF SURFACE MODIFIED CERAMICS

D. J. Green
College of Earth and Mineral Sciences
Phone: (814) 863-2011

$98,593 01-2

Modification of surface layers of ceramics to introduce surface compression and increase hardness and fracture toughness of transformation-toughened ZrO₂ and Al₂O₃. Surface infiltration when ceramic is pressed or partially sintered. Development of a second phase surface layer during final densification. Indentation cracking used to study crack nucleation and growth and determine fracture toughness. Stress and composition profiles determined by NSLS X-ray diffraction data.
452. TWIN BOUNDARIES AND HETEROFASE INTERFACES IN FERROELASTIC MARTENSITES

G. R. Barsch
Materials Research Laboratory
Phone: (814) 865-1657

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

453. GRAIN BOUNDARY AND SURFACE DIFFUSION IN OXIDE SYSTEMS

V. S. Stubican
Dept. of Materials Science and Engineering
Phone: (814) 865-9921

This research addresses diffusional transport phenomena on ionic surfaces and grain boundaries. Specifically, studies of surface diffusion of $^{51}$Cr on MgO and $^{57}$Co on MgO and NiO, and grain boundary diffusion of $^{59}$Fe in Fe$_3$O$_4$. 

454. EXPERIMENTAL AND THEORETICAL STUDIES ON TRANSPORT PROCESSES IN LASER WELDING

T. DebRoy  
Dept. of Materials Science and Engineering  
Phone: (814) 865-1974  
$71,326 01-5

Modeling of solute loss, heat transfer and fluid flow during laser welding of stainless steels. Calculation of local temperature profile, weld pool velocity and vaporization of alloying elements, correlative experimental determination of weld microstructure and chemistry, time resolved emission spectroscopic measurements to determine composition of metal vapors.

455. LASER PROCESSING OF CERAMICS

G. L. Messing  
Dept. of Materials Science and Engineering  
Phone: (814) 865-2262  
$63,000 01-5

Correlations between melt crystallization kinetics, thermodynamics, phase equilibria, etc., during rapid solidification of Al2O3-SiO2 compositions around the mullite phase field and Al2O3-ZrO2 both melted with a 10.6 micron CO2 laser. Preparation of ceramic powders using rapid solidification processing by injecting solutions and/or solid particles coaxially into a plasma flame. Investigation of morphological modification by single particle melting and rapid solidification, calcination of oxide precursors and rapid reaction of multicomponent systems. Formation and properties of mullite powders with respect to phase equilibria, plasma parameters, and solidification conditions.

456. GAS SURFACE INTERACTION USING PULSED-LASER ATOM-PROBE FIELD ION MICROSCOPY

T. T. Tsong  
Dept. of Physics  
Phone: (814) 865-2813  
$68,000 02-2

Experimental investigation of surface catalyzed chemical reactions using pulsed laser time-of-flight atom probe field ion microscopy. Field adsorbed H3 will be studied on various crystalline surfaces of various metals and alloys. Desorbed ion species such as H+, D+, H2+, HD+, D2+, H3+, H2D+, and D3+ as a function of tip temperature, tip material, and field strength to determine associative and dissociative mechanisms of hydrogen on various surfaces. Other reactions include methanation of CO and reduction of NO. Adsorption of atoms and molecules on a surface induced by an applied
Synthesis and characterization of crystalline materials formed at low temperatures. The objective is to apply some of the very new and exciting advances in chemically-bonded ceramics to making much stronger and more impermeable materials that can be processed at low temperatures. The material have potential application as low-level radioactive waste hosts.

Study of the staging phenomenon in graphite intercalation compounds (principally with Li) and other layer systems by X-ray and neutron diffraction. Independent variables are temperature, hydrostatic pressure and concentration of alkali metal intercalate. Experimental determination of the staging temperature vs. concentration phase diagram. Elucidation of new high-pressure phases. Determination of the nature, origin, and consequences of stage disorder. Investigation of kinetics of staging transitions with emphasis on identifying metastable structures.
Atomistic computer simulations to investigate the relationship between the structure of grain boundaries and segregation propensity, the structural changes provoked by the segregation and their effect on boundary behavior, and the transformation of the boundary structures associated with segregation and structural multiplicity. Calculations on segregation propensity for tilt boundaries in iron with Sn, Sb, and Cu as impurities and for twist boundaries in copper with Bi as an impurity. Temperature effects in structural transformations of grain boundaries are investigated by calculating the entropy contributions to the free energy. In addition to the development of semiempirical schemes for describing interatomic forces in the form of pair potentials, a quantum mechanical tight-binding approach to the structural studies of grain boundaries and cohesion at interfaces will be investigated.

Initiation of slow crack growth in polyethylene, ethyleneoctene copolymers with various octene concentrations branch densities of 2-10 per 100 carbon atoms and narrow molecular weight distribution. Measurement under plane strain of rate of formation of damaged zone at root of a notch as function of stress, time, temperature, notch depth, specimen geometry. Characterization of extent of porous, fibrillated and fractured regions which constitute the damaged zone using optical microscopy, SEM, and TEM. Determination of constitutive equations for various regions of damaged zone. Use of data to construct a mathematical model based on the micro-mechanics of fracture for predicting long time failure in engineering structures.
UNIVERSITY OF PENNSYLVANIA (continued)

461. FUNDAMENTALS OF HARDENING AND DECOHESION BEHAVIOR IN TIME-DEPENDENT CYCLIC DEFORMATION

C. Laird
Dept. of Materials Science and Engineering
Phone: (215) 898-6664

J. L. Bassani
Phone: (215) 898-5632

$117,000 01-2

Role of hardening on active and latent slip systems on the deformation of metals under monotonic and cyclic loading; characterization of dislocation structure developed in Cu during time-dependent and time-independent deformation; formulate a physically realistic micromechanical description of the deformation; single crystal behavior followed by polycrystalline materials studies on Cu, Cu-O, and Cu-Pb alloys; cyclic creep deformation and fracture and the role of non-metallic particles on cavity formation and linkage.

462. INTRINSIC SURFACE PHONONS ON RECONSTRUCTED SEMICONDUCTOR SURFACES

E. J. Mele
Dept. of Physics
Phone: (215) 898-3135

$88,745 (17 months) 02-3

Theoretical study of the lattice dynamics of reconstructed semiconductor surfaces. Relation between localized surface electronic and surface structural and vibrational properties. Computation scheme combines a short range elastic Hamiltonian with a static electronic polarization extracted from a tight binding representation of the valence electronic bands. Applications include models of Si(100)2x1 and Si(111)2x1 surfaces and generalization of the results to deduce a structural Hamiltonian for Ge.
463. MICROCHEMISTRY ANALYSIS OF POLYCRYSTALLINE Ni$_3$Al AND OTHER ORDERED ALLOYS USING THE FIELD-ION MICROSCOPE ATOM PROBE

S. S. Brenner  
Dept. of Metallurgical and Materials Engineering  
Phone: (412) 624-5445  
$115,971  

Investigation of structure and microchemistry of grain boundaries in Ni$_3$Al containing different Ni/Al stoichiometric ratios, substitutional solutes, and grain boundary B concentrations. Principal analytical methods involve the field-ion microscope atom probe. Other variable parameters include grain-boundary orientation, bulk B concentration, Al substoichiometry, and comparison between cast and melt-spun Ni$_3$Al-B material.

464. HIGH TEMPERATURE CORROSION OF CERAMICS

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Dept. of Metallurgical and Materials Engineering  
Phone: (412) 624-5300  
J. R. Blachere  
Dept. of Metallurgical and Materials Engineering  
Phone: (412) 624-5300  
$49,999  

Thermodynamic and kinetic analyses of gaseous and molten salt corrosion of oxides (SiO$_2$, Al$_2$O$_3$, Cr$_2$O$_3$, and ZrO$_2$) in oxidizing, sulfidizing, and reducing environments, thermogravimetric measurement of corrosion kinetics. Gas mixtures of SO$_2$-SO$_3$-O$_2$, H$_2$-H$_2$O, and CO-CO$_2$-O$_2$ at temperatures in the interval 700$^\circ$C to 1400$^\circ$C. Effects of deposits such as Na$_2$SO$_4$, NaOH, and Na$_2$CO$_3$ on the gas-induced corrosion. Mechanisms of corrosion of high purity materials and of materials with microstructures and impurities characteristic of advanced commercial materials. Morphology of the corrosion products.
UNIVERSITY OF PITTSBURGH (continued)

465. THE PHYSICS OF PATTERN FORMATION AT LIQUID INTERFACES

J. V. Maher
Dept. of Physics and Astronomy
Phone: (412) 624-0872

$94,283 02-2

Studies of the physics of binary liquid interfaces. Experiments on onset and nonlinear growth of hydrodynamic instabilities, nonlinear pattern formation, and transition to turbulence. The diffusion-driven instability of a quenched liquid interface and the Saffman-Taylor instability (viscous fingering) investigated with careful control over such parameters as density difference, viscosity difference, and interfacial tension. Light scattering investigations of the dynamics of phase separation for a binary liquid mixture imprisoned in a gel to understand the role of hydrodynamics.

PRINCETON UNIVERSITY
Princeton, NJ 08544

466. THE FORMATION OF ORDERED MICROSTRUCTURES BY SLIP CASTING AND RELATED PROCESSES

W. B. Russel
Dept. of Chemical Engineering
Phone: (609) 452-4590

$70,278 01-3

The dynamics of three processes (sedimentation, ultrafiltration, and slip casting) which concentrate small particles from a dilute solution, with particular emphasis on the structure of the resulting dense phase as a function of the processing conditions. Objectives are to define the range of conditions which produce an ordered casting, develop process models, and perform measurements of diffusion models in dense suspensions. Modeling to involve the formulation and solution of a macroscopic conservation equation governing the mean volume fraction, coupled to a microstructural equation describing the relaxation of imperfections enroute to the equilibrium ordered state. Dynamic light scattering experiments on concentrated silica dispersions to determine diffusion coefficients. Sedimentation and ultrafiltration experiments following the formation of both disordered and ordered phases.
PRINCETON UNIVERSITY (continued)

467. MODULATED INFRARED LINEAR DICHROISM STUDIES OF THE DYNAMICS OF MOLECULAR ORIENTATION AND RELAXATION IN POLYMERS

J. T. Koberstein
Dept. of Chemical Engineering
Phone: (609) 452-5721
R. K. Prud’homme
Dept. of Chemical Engineering
Phone: (609) 452-4577

$84,000 (18 months) 03-01

Examination of the fundamental relationship between chain confirmational changes and the macroscopic material responses during deformation. The program is based on the coupling of rheological and rheo-optical measurements during well characterized deformations. An in-situ infrared dichroism technique is used to study dynamically the molecular orientation during chain deformation and relaxation. Novel specimens that are partially deuterated allow the characterization of the deformation and relaxation behavior of essentially any segment of a polymer chain.

468. ASPECTS OF PHOTOIONIZATION OF IMPURITIES AND ELECTRON TRANSFER IN IONIC CRYSTALS

D. S. McClure
Dept. of Chemistry
Phone: (609) 452-4980

$86,600 03-1

Research of the relationship between the energy levels of impurity ions and the energy levels in the host crystal. Photoionization thresholds of impurity ions in crystals, such as Sm$^{2+}$ in SrF$_2$, BaF$_2$, and CaF$_2$. Two photon spectroscopy in the strongly coupled ion-lattice system, MgO:N$i^{+2}$. Studies of trapped excitons and phototransfer of electrons from one impurity ion to another.
Examination of the possibility of obtaining glasses with a relatively high conductivity in which the charge carrier is a divalent cation. Target systems include $\text{MI}_2\text{-M(PO}_3\text{)}_2\text{/M(PS}_3\text{)}_2$, where $\text{M}^{2+}$ is Pb$^{2+}$, Cd$^{2+}$, or Sn$^{2+}$. Characterizations include measurements of electrical conductivity, nuclear magnetic resonance, internal friction, visco-elastic properties, and glass transition temperatures. Correlation of mechanical and electrical phenomena in mixed conduction systems such as mixed Pb(PO$_3$)$_3$-PbBr$_2$-PbCl$_2$ glasses and Na vanadate glasses.

This grant supports MATRIX, a group of 20 scientists from 9 institutions who have common interests in utilizing X-ray synchrotron radiation for unique materials research. This group has available to it a specialized beam line at the National Synchrotron Light Source, NSLS. A unique and versatile monochromator provides radiation to a four-circle Huber diffractometer for the basic system. Multiple counting systems are available as well as a low temperature stage, a high temperature stage, and a specialized surface diffraction chamber. The funds requested are to cover the operational expenses of this beam line at NSLS for all MATRIX members and to support part of the research on phase transformation studies and X-ray surface and interface studies.
471. MECHANISMS OF ELEVATED TEMPERATURE RUPTURE IN SINGLE PHASE CERAMICS

A. A. Solomon
School of Nuclear Engineering
Phone: (317) 494-5753

$91,250 (23 months) 01-2

Study of elevated temperature tensile creep and stress rupture in well-characterized single phase ceramics in terms of rate controlling mechanisms and microstructural evolution. Experimental techniques consist of (1) tensile creep using constant true stress, (2) internal pressurization of pores with inert insoluble gas and microscopic measurement of pore or cavity growth under known hydrostatic pressure and surface tension driving forces. Results are correlated with quantitative microstructural studies of porosity evolution. Materials under investigation are CoO, UO₂, NiO, carbonyl Ni, and Si₃N₄.

472. ZERO-FLUX PLANES AND FLUX REVERSALS IN MULTICOMPONENT DIFFUSION

M. A. Dayananda
School of Materials Engineering
Phone: (317) 494-4113

$77,000 01-3

The objectives are (1) to explore the role and development of zero-flux planes (ZFP) and flux reversals in both single phase and multiphase diffusion couples in multicomponent systems during isothermal diffusion, (2) to characterize the ZFP compositions in terms of diffusion paths and thermodynamic data, (3) to study the feasibility of regulating the interdiffusion of elements with preferential development of ZFPs. Zero flux planes for individual components within the diffusion zone of either a single or multiphase multicomponent system have been identified. At ZFPs the interdiffusion flux of a given component goes to zero and exhibits reversal in its flow direction on either side of the plane.
473. STUDY OF MULTICOMPONENT DIFFUSION AND TRANSPORT PHENOMENA

H. Sato
School of Materials Engineering
Phone: (317) 494-4096
R. Kikuchi
School of Materials Engineering
Phone: (317) 494-4099

$96,026 01-3

Research on multicomponent diffusion under general chemical potential gradients. Application of the path probability method of irreversible statistical mechanics to analytically derive the Onsager relations for diffusion on an atomistic basis. The conditions treated are general enabling relations among measurable quantities under a variety of driving forces such as the Nernst-Einstein relation and the Haven ratio in multicomponent systems, to then be clearly understood. The general formalism of multicomponent diffusion and cross terms in the Onsager relations is examined, and the role of apparent vacancy flows and "wind" effects investigated. The method is applied to chemical diffusion problems in multicomponent systems and to understanding established empirical concepts such as "diffusion path" and "zero flux planes."

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

J. G. Mullen
Dept. of Physics
Phone: (317) 494-3031

$57,000 02-2

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

R. G. Reifenberger
Dept. of Physics.
Phone: (317) 494-3032

Interaction of visible and near-UV laser light with sub-micron metallic surfaces and with adatoms or adsorbates. Electrons from field emission tips are photo-emitted by a focused Argon-ion laser beam tuned to a particular wavelength and tunnel into vacuum through a surface potential barrier which is distorted by a strong applied electric field. The final state energy distribution analyzed for influence of electronic structure, of the quantum mechanical transmission through the barrier, and of the nature of photoexcitation at photon energies below the barrier top. Thermal effects of laser heating, laser assisted diffusion and laser induced desorption of adatoms.

RENSSELAER POLYTECHNIC INSTITUTE
Troy, NY 12181

476. TESTS AND MODELING FOR SINTERING THEORY

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Dept. of Materials Engineering
Phone: (518) 266-6373

R. M. German
Dept. of Materials Engineering
Phone: (518) 266-6445

Research on multicomponent diffusion under general chemical potential gradients. Application of the path probability method of irreversible statistical mechanics to analytically derive the Onsager relations for diffusion on an atomistic basis. The conditions treated are general enabling relations among measurable quantities under a variety of driving forces such as the Nernst-Einstein relation and the Haven ratio in multicomponent systems, to then be clearly understood. The general formalism of multicomponent diffusion and cross terms in the Onsager relations is examined, and the role of apparent vacancy flows and "wind" effects investigated. The method is applied to chemical diffusion problems in multicomponent systems and to understanding established empirical concepts such as "diffusion path" and "zero flux planes."
MECHANISM OF MECHANICAL FATIGUE IN FUSED SILICA

M. Tomozawa  
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STUDY OF THE KINETICS AND THERMODYNAMICS OF HYDROGEN IN PD-BASED ALLOYS

R. B. McLellan  
Dept. of Mechanical Engineering and Materials Science  
Phone: (713) 527-4993  

Systematic measurements of the solubility, thermodynamic properties, and diffusivity of H atoms in the same Pd-based binary alloys. Low (270-350K) and high (500-1000K) temperature diffusion measurements respectively by a double-cell electrolyte system and the permeability time-lag method. Measurement of the temperature and pressure dependence of hydrogen solubility and the temperature and the substitutional solute concentration dependence of the elastic constants. Magnetic susceptibility and elastic constant measurements for Pd and Pd alloys. Statistical thermodynamic modeling. Theoretical models based upon Thiele moment expansions and cell cluster techniques for interstitial solid solutions containing secondary defects (e.g., vacancies).
479. APPLICATION OF SPIN-SENSITIVE ELECTRON SPECTROSCOPIES TO INVESTIGATIONS OF ELECTRONIC AND MAGNETIC PROPERTIES OF SOLID SURFACES AND EPITAXIAL SYSTEMS

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Physics Dept.
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F. B. Dunning
Dept. of Physics
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Spin polarized beams of electrons and metastable He(23S) atoms used in studies of surface magnetic behavior, dynamics of metastable deexcitation at surfaces, electronic properties of absorbed layers. Spin Polarized Low Energy Electron Diffraction (SPLLED) and Metastable Deexcitation Spectroscopy (MDS) investigations of magnetic properties of epitaxial systems at the monolayer level. Emphasis on monolayers of Cr on Au(110), and monolayers of V and Fe on Ag(001) for which theory predicts strongly enhanced two-dimensional ferromagnetic moments on metallic overlayers, interfaces and superlattices.

480. FRACTURE TOUGHNESS OF MATERIALS

S. J. Burns
Dept. of Mechanical Engineering
Phone: (716) 275-4082

Research on the relationships between deformation processes and phase transformations occurring at the tips of cracks and the fracture toughness of materials. Specific activities include observations of deformation structures at the tips of cracks in single crystals of LiF and Si, analysis of dislocation nucleation from tips of macroscopic cracks in a high-strength steel using crack-tip shields for the position of dislocations relative to the tips of cracks, thermomechanical measurements of phase transitions in ZrO2 for phase transformation fracture toughening, and a thermodynamic analysis of thermal expansivity in materials.
481. MICROSTRUCTURAL BEHAVIOR OF NON-EQUILIBRIUM SYSTEMS

J. C. M. Li
Dept. of Mechanical Engineering
Phone: (716) 275-4038
$120,004 01-2

Coupled theoretical and experimental research on amorphous metals. Topics include: a) vacancies and interstitials introduced by energetic atoms, b) negative creep induced by a positive stress, c) crack extension and dislocation emission, and d) nucleation events in melting. Research also includes studies of rapidly crystallized structures.

482. ADVANCED Si₃N₄ SYSTEM STUDIES

P. E. D. Morgan
Phone: (805) 373-4273
$224,924 01-5

Investigations of Si-S chemistry to provide starting points for the preparation of Si₃N₄ and SiC in various forms such as powder, whiskers, fibers, etc. Room temperature reactions of SiS₂ with hydrazine. TGA, XRD, TEM, NMR, IR, Fracture toughness.

483. LOCAL STRUCTURE OF METAL ATOMS IN SILICA AND SILICATES

S. H. Garofalini
Dept. of Ceramics
Phone: (201) 932-2216
$26,164 01-3

Local structure and bulk and surface diffusion of metal ions in vitreous silica and silicated glasses are investigated using a combination of X-ray extended fine structure (EXAFS) measurements and computer simulations using molecular dynamics methods. Studies include the effects of local structure, interatomic potential functions, atom size, ion clustering, and sample preparation on the mobility of metal species. Systems include alkali-zinc-silicates, sol-gel-prepared zinc silicates, and platinum on silica.
RUTGERS UNIVERSITY (continued)

484. HIGH PRESSURE AND SYNCHROTRON RADIATION STUDIES OF SOLID STATE ELECTRONIC INSTABILITIES

J. H. Pifer
Dept. of Physics
Phone: (201) 932-2524
M. C. Croft
Dept. of Physics
Phone: (201) 932-2522

$139,200 02-2

Studies of the configurational instabilities in 3d, 4f, and 5f compounds utilizing a novel high pressure diamond anvil electron paramagnetic resonance apparatus capable of operating at 100 kbar at liquid helium temperatures. Resistivity measurements and core level X-ray absorption studies using synchrotron radiation on both crystalline and amorphous mixed valence materials. Research on the ThCr₂Si₂ structure materials, with Th replaced by Ce and Eu to investigate the interplay of rare earth valence state with p-p bond formation. Investigation of heavy fermion regime with Cr replaced by Mn₁₋ₓCrₓ. New amorphous rare earth compounds in thin films. Valence charge study of Ce in Ce(RhₓPd₁₋ₓ)₃.

SETON HALL UNIVERSITY
South Orange, NJ 07079

485. THE USE OF SURFACE CHARACTERIZED DISPERSED METAL CATALYSTS IN CATALYTIC REACTIONS

R. L. Augustine
Dept. of Chemistry
Phone: (201) 761-9033

$63,500 03-3

Extension of the single turnover reaction sequence developed for the surface characterization of Pt/CPG catalysts to characterize other catalysts and support combinations. The effects of the support on site specific reactivity will be determined. Support materials studied include alumina, silica, and titania. Metals studied include platinum, palladium, and rhenium.
486. CHARACTERIZATION OF PORE EVOLUTION IN CERAMICS DURING CREEP FAILURE AND DENSIFICATION

R. A. Page
Dept. of Materials Science
Phone: (515) 684-5111 X3252

J. Lankford
Dept. of Materials Science
Phone: (515) 684-5111 X2317

$154,000

Characterization of pore evolution during sintering and cavitation during creep. Creep studies concerned with the effect of grain size, grain boundary phases, and choice of ceramic material with emphasis on compressive creep cavitation. Characterization of the effect of grain size and grain boundary chemistry upon the cavitation of pure Al2O3 subject to uniaxial tensile stress. Characterization of cavity development and breakaway conditions during the final stage sintering of Al2O3. Small angle neutron scattering to yield cavity nucleation and growth rates and average pore size, distribution, and morphology. TEM and precision density characterization. Modeling of cavitation and sintering behavior. Principal experimental materials: Al2O3, SiC.

487. MINOR ALLOYING ELEMENTS IN THE PITTING BEHAVIOR OF METALS AND ALLOYS

D. D. Macdonald
Chemistry Laboratory
Phone: (415) 859-3195

$128,908

Experimental and theoretical investigation of pitting in austenitic stainless steels (Fe-Cr-X-base composition). Extension of the solute/vacancy interaction model to consider breakdown of passive films and role of minor alloying elements thereon, modeling rate of generation of cation vacancies at the film/solution interface and the interaction between the solutes and vacancies for various solute types (effective valence and concentration). Experimental studies of breakdown characteristics of various alloys in aqueous chloride solutions and possibly other electrolytes. Application of results to alloy design.
488. INTERNAL-VARIABLE BASED MODELS FOR ELEVATED TEMPERATURE FATIGUE AND DEFORMATION

A. K. Miller  
Dept. of Materials Science and Engineering  
Phone: (415) 723-3732  

$190,476 01-2

A program of research to develop a new unified computer model for elevated-temperature fatigue that will be based upon explicit representations of the controlling internal physical processes, and which will be completely quantitative and computer-based. Related research on the development of a physically-based model of the deformation and ductile failure behavior of metals and alloys, including development of improved constitutive equations for multiaxial plasticity, and a new model for sheet metal formability under nonproportional strain paths. This research advances earlier modeling work (the development of MATMOD and MATCON constitutive relations) on the plasticity of materials and serves as input to the elevated-temperature fatigue model.

489. MECHANISMS OF HIGH TEMPERATURE CRACK GROWTH IN METALS AND ALLOYS

W. D. Nix  
Dept. of Materials Science and Engineering  
Phone: (415) 497-4259  

$98,619 (5 Months) 01-2

Study of the processes of creep crack extension in simple metals (Cu and Ni), examination of cavitation damage at crack tips using implanted intergranular cavities and intergranular segregation of Sb in Cu to permit grain boundary fracture in post-creep impact tests, study of the driving forces for crack growth and the temperature dependence of the growth process, examination of the effects of environments on creep crack growth in Ni alloys containing carbon, study of creep crack growth in 304 stainless steel containing different intergranular carbide distributions, theoretical studies of cavitation and crack growth.
STANFORD UNIVERSITY (continued)

490. PHOTOELECTRONIC PROPERTIES OF II-VI HETEROJUNCTIONS

R. H. Bube
Dept. of Materials Science and Engineering
Phone: (415) 497-2534

$210,000 01-3

Interactions occurring at the interface between CdTe with other materials, and the role of interfacial microstructure and microchemistry on the electrical properties of such CdTe containing heterojunctions. Effects of etching and heat treatment on surfaces, Schottky barriers, and heterojunctions formed on CdTe, and the preparation and behavior of polycrystalline films of CdTe. Grain boundary characterization and passivation. Measurements include J-V curves in dark and light; junction capacitance; surface photovoltage; Schottky-barrier formation; spectral response; and diffusion lengths. Scanning transmission electron microscopy and high resolution and electron microdiffraction; XPS, Auger analysis; vacuum evaporation; spray pyrolysis; rf sputter deposition; magnetron sputtering; and chemical vapor deposition; and closed-space vapor transport techniques.

491. A STUDY OF MECHANICAL PROCESSING DAMAGE IN BRITTLE MATERIALS

B. T. Khuri-Yakub
Dept. of Electrical Engineering
Phone: (415) 497-0718

$102,701 01-5

The proposed research will investigate machining damage in brittle materials, initially hot-pressed Si$_3$N$_4$, and the associated residual surface stresses. Nondestructive evaluation (NDE) techniques will be developed and applied to the measurement of the depth of shallow cracks, simulating machining damage, and local stress fields. An attempt will be made to correlate the damage with microstructural features and to determine a quantitative relation between damage and remaining strength.
492. THE USE OF NON-DESTRUCTIVE EVALUATION TECHNIQUES IN THE STUDY OF SMALL FATIGUE CRACKS

D. V. Nelson
Dept. of Materials Science and Engineering
Phone: (415) 497-2123

J. C. Shyne
Dept. of Materials Science and Engineering
Phone: (415) 497-2123

$130,000 01-5

Study of the growth behavior of fatigue microcracks in 4140 and 300 M steels, as influenced by different microstructures. Monitoring of crack depth and variation in crack closure stress with crack growth using surface acoustic waves as a probe. Comparison of closure stress behavior with that determined by SEM measurements of crack mouth opening displacement vs. applied stress. Measurement by X-ray diffraction of changes in surface residual stresses during fatigue cycling. Correlation of crack growth rate with closure stress behavior, at different stress amplitudes and two mean stress levels. Investigation of the use of an acoustic microscope technique to furnish quantitative information about residual stresses.

493. A QUEST FOR A NEW SUPERCONDUCTING STATE

J. P. Collman
Dept. of Chemistry
Phone: (415) 497-4648

W. A. Little
Dept. of Physics
Phone: (415) 497-4233

$100,000 03-1

Synthesis and characterization of organic conductors in which the conducting spine is encompassed by macrocyclic dyes. Experimental tests of excitonic superconductivity. Preparation of polymeric materials consisting of stacked or bridged-stacked metalloporphyrin or metallophthalocyanine complexes. Structural characterization using EXAFS and XANES at the Stanford Synchrotron Radiation Laboratory and X-ray powder and single crystal crystallography. Measurements of conductivity, photoconductivity, and magnetic susceptibility. Calculations using extended Hückel molecular and band theory.
494. SPIN POLARIZED PHOTOELECTRON STUDIES OF MAGNETIC IN SOLIDS

G. M. Rothberg
Dept. of Materials and Metallurgical Engineering
Phone: (201) 420-5269
$ 96,000 02-2

Magnetic order and the spin dependence of electron scattering in solids by means of a new technique, Spin Polarized Extended X-ray Absorption Fine Structure, or SPEXAFS. The spin polarization of electrons from exchange-split photoemission peaks used to observe EXAFS and obtain information about the distance and temperature dependences of spin-spin correlations in magnetic solids and on surfaces. Features of the photoelectron spectrum used such as ordinary EXAFS and the plasmon-loss peaks to obtain additional information. Photoemission EXAFS has a unique chemical sensitivity that make possible in Al-O systems the study of the atomic structure around an element in different chemical environments.

495. THE CATALYTIC REACTIVITY TO THIN FILM CRYSTAL SURFACES

R. W. Vook
Dept. of Physics
Phone: (315) 423-2564
J. A. Schwarz
Dept. of Chemical Engineering and Materials Science
Phone: (315) 423-4575
$171,607 01-1

Characterization of topography and defect structure on thin film surfaces (Pd, Pt) and of factors that determine their chemical reactivities, measurement of adsorption and desorption (thermal and electron beam induced) kinetics of O2, CO, and hydrocarbons on these films, work function determination upon gaseous adsorption as a function of surface topography and defect structure, comparison of reactivities of vapor deposited thin film surfaces with similar surfaces that were sputter etched and annealed, chemical reaction investigations at elevated pressures using thin film samples as prototype catalysts that include the effects of catalytic promoters and poisons, techniques used - LEED, AES, EELS, TPD, TEM/TED, RHEED, work function.
496. STATISTICAL MECHANICS OF POLYMER SYSTEMS

J. Kovac
Dept. of Chemistry
Phone: (615) 974-3444

Theoretical investigation into the equilibrium and dynamic behavior of amorphous polymers over a broad range of concentration, molecular weight, and temperature. The investigations involve non-equilibrium thermodynamics, equilibrium and non-equilibrium statistical mechanics, and computer simulation. Specific problems include more realistic models for single chain dynamics, conformation and dynamics of chains in semi-dilute and bulk systems and equilibrium and dynamic aspects of the glass transition.

497. EXPERIMENTAL STUDIES OF THE ELECTRONIC STRUCTURE OF I-II AND I-III INTERMETALLIC COMPOUNDS

I. M. Curelaru
Dept. of Materials Science and Engineering
Phone: (801) 581-4850, 3161

Systematic investigation of the electronic structure of the occupied and empty states for I-II and I-III intermetallic Zintl compounds, with concern for the significance of nonstoichiometry, defect lattice, and degree of localization of conduction orbitals in determining physical behavior. Spectroscopic techniques consist of X-ray photoelectron spectroscopy (XPS), electron energy loss spectroscopy (EELS), core ionization loss spectroscopy (CILS), appearance potential spectroscopy (APS), and extended appearance potential fine structure (EAPFS). Comparison of XPS, EELS, CILS, and data with existing LCAO, cluster model, and self-consistent linear muffin tin LMT band-structure calculations.
UNIVERSITY OF UTAH (continued)

498. FABRICATION, PHASE TRANSFORMATION STUDIES AND, CHARACTERIZATION OF SIC-ALN-AL₂OC CERAMICS

A. V. Virkar  
Dept. of Materials Science and Engineering  
Phone: (801) 581-5396

R. Gohil  
Dept. of Materials Science and Engineering  
Phone: (801) 581-3781

$109,642 01-1

Preparation of SiC-AlN-Al₂OC powders by a carbothermal reaction of a mixture of SiO₂ and Al₂O₃ in N₂ or Ar. Fabrication of SiC-AlN-Al₂OC ceramics by hot pressing, and subjecting such dense, hot pressed ceramics to various annealing treatments. X-ray diffraction and STEM analysis to investigate phase equilibria, precipitate morphology, spinodal decompositions and grain boundaries especially with special regard to the nucleation and growth of possible grain boundary phases. Evaluation of room temperature bend strength and fracture toughness and elevated temperature creep. Emphasis on understanding the inter-relationship of fabrication, microstructure, and mechanical behavior.

499. THEORETICAL AND EXPERIMENTAL STUDY OF SOLID PHASE MISCIBILITY GAPS IN III/V QUATERNARY ALLOYS

G. B. Stringfellow  
Dept. of Materials Science and Engineering  
Phone: (801) 581-8387

$95,903 01-3

Development of an understanding of miscibility gaps in alloys including organometallic vapor phase epitaxial growth of metastable alloys. Effect of short range (100A to 1000A) clustering compositional inhomogeneity in GaAs₀.₆Sb₀.₄ alloys on hole and electron mobility and photoluminescence half-widths. Raman spectroscopy and STEM analysis of spinodal compositions and clustering.
B-95

VIRGINIA COMMONWEALTH UNIVERSITY
Richmond, VA 23284

500. INTERNATIONAL SYMPOSIUM ON THE PHYSICS AND CHEMISTRY OF SMALL CLUSTERS

P. Jena
Department of Physics
Phone: (804) 257-1313

$5,000 01-1

International symposium to be held on physics and chemistry of small clusters. Fundamental aspects of the structural, thermodynamic and electronic properties of small clusters will be examined. Discussions of practical applications will be included.

UNIVERSITY OF VIRGINIA
Charlottesville, VA 22901

501. STUDY OF THE EMBEDDED ATOM METHOD OF ATOMISTIC CALCULATIONS FOR METALS AND ALLOYS

R. A. Johnson
Department of Materials Science
Phone: (804) 924-6356

$73,200 01-1

Theoretical studies to (1) obtain a better physical insight into the relationship between the input data and the EAM model parameters, (2) study the effects which variation of the EAM model parameters have on predicted material properties, and (3) use these results to assess the range of applicability of the EAM model and to improve its reliability within this range.

502. MICROSTRUCTURAL EFFECTS ON THE FATIGUE BEHAVIOR OF FE-C-X ALLOYS

G. L. Shiflet
Dept. of Materials Science
Phone: (804) 924-6340

E. A. Starke Jr.
Dept. of Materials Science
Phone: (804) 924-6340

$81,717 01-2

This research project addresses the cyclic fatigue behavior of low alloy multiphase steels. The program will aim to establish the effect of microstructure on crack initiation and propagation in tensile and fatigue tests of steels with well-controlled and characterized microstructures. Parallel modeling of the phase stability and crack propagation is planned.
A scanning tunneling microscope (STM), operating at liquid nitrogen temperature, used to image atoms at surfaces of layer structure crystals and to detect the electronic rearrangement due to charge-density waves (CDW's). Further instrument development, and study of a wider range of CDW transitions. More detailed information on the CDW structure and how it modifies the STM image. Development of a similar instrument operating at liquid helium temperatures for the study of both CDW and superconducting transitions. Surface structure, defects and the early stages of oxidation using both instruments. Development of techniques for imaging surface absorbed molecules and eventual vibrational spectroscopy of such molecules. Continuing experiments on standard tunnel junctions using the STM to study the early stages of oxide and doped oxide barrier formation. STM studies to elucidate the localized atomic and localized electronic structure at surfaces and interfaces.

Theoretical investigation of the influence of magnetic impurities on the critical magnetic field $H_{c2}$ and other physical properties. Special attention given to the Chevrel phase superconductors and to the newly discovered material phases displaying field induced superconductivity. Emphasis on mechanisms to enhance high field behavior of superconductors. The response of charge density waves to electric and magnetic fields. Study of charge density waves in certain heavy Fermion systems.
505. NON-EMPirical INTERATOMIC POTENTIALS FOR TRANSITION METALS

A. E. Carlsson
Dept. of Physics
Phone: (314) 889-5739

$42,000 (16 months) 02-2

Development of existing scheme for calculating interatomic potentials in simplified tight-binding models into a method applicable to transition metals and transition metal alloys with defects. Consideration of tight-binding models, the tight-binding parameters from a first principles band theory, and effects beyond the extant tight-binding model. Interatomic potentials tested both by experimental data and band theoretic calculations for surfaces and vacancies and subsequently used to calculate the properties of dislocations and grain boundaries.

506. X-RAY SPECTROSCOPY OF SOLIDS UNDER PRESSURE

R. L. Ingalls
Dept. of Physics
Phone: (206) 543-5900

$107,000 (15 months) 02-2

Investigation of the structure and behavior of materials at high pressure by measuring the Extended X-ray Absorption Fine Structure (EXAFS) utilizing synchrotron radiation. Focus on the behavior of materials exhibiting the mixed valent insulator-to-metal transformation, clearly apparent in their X-ray absorption spectra. Examination of the X-ray Absorption Near Edge Structure (XANES) in such materials, as well as others with pressure-sensitive phase transformations. Experiments at the Stanford Synchrotron Radiation Laboratory.
UNIVERSITY OF WASHINGTON (continued)

507. FUNDAMENTAL STUDIES OF ELASTOMERS

B. E. Eichinger
Dept. of Chemistry
Phone: (206) 543-1653

$103,500 03-1

Chemistry and physics of high elasticity aimed towards an improved understanding of the properties of elastomers. The approach uses experimental, computational, and theoretical methods to investigate the relationship between network structure, viscoelastic behavior, and equilibrium properties. Networks that are cross-linked through coordination complexes are being produced, they will be used for a variety of studies, including small angle X-ray scattering and stress-strain measurements. Computer simulations of network formation are used to investigate the statistics that govern the microstructural features of elastomers. The theory of the shape distribution of polymer molecules is being developed in conjunction with a theory of the elastic free energy.

WEST VIRGINIA UNIVERSITY
Morgantown, WV 26506

508. ELECTRON HYBRIDIZATION EFFECTS AND THE CRYSTAL STRUCTURE OF PLUTONIUM

B. R. Cooper
Dept. of Physics
Phone: (304) 293-3423

$61,000 03-1

Investigation of the crystallographic allotropes of elemental plutonium with detailed calculations of the electronic structure, including correlation effects and contributions to the lattice energy. Theoretical model based on hybridization of the 5f electrons with the band electrons. Studies of plutonium mon pnictides and monochalcogenides, the plutonium alpha distorted fcc phase, magnetic ordering, electrical resistivity, and self-consistent surface electronic structure.
509. STUDIES OF ALTERNATIVE-CRYSTALLIZATION-PHASE NUCLEATION

T. F. Kelly
Dept. of Metallurgical and Mineral Engineering
Phone: (608) 263-1073
$95,950 (15 months) 01-1

Liquid-to-crystal nucleation theory to predict which of several crystalline phases will solidify from small droplets of metal alloys. An experimental program to produce and characterize these alternative crystallization phases. Droplet processing by electrohydrodynamic atomization, centrifugal atomization, and levitation melting. Thermal analysis and analytical electron microscopy of as solidified droplets. Comparison of experimental findings with predictions of liquid-to-crystal nucleation theory.

510. THE STABILITY OF AMORPHOUS METALS ON SEMICONDUCTOR SUBSTRATES

J. D. Wiley
Dept. of Electrical and Computer Engineering
Phone: (608) 263-1643

J. H. Perepezko
Dept. of Metallurgy and Mineral Engineering
Phone: (608) 263-1678
$87,340 01-1

Experimental investigation of the structure, stability, and atomic transport behavior of high-T amorphous-metal films on semiconductor substrates. RF sputtering deposition of thin amorphous films of Ni-Nb, Mo-Si, and W-Si alloys on semiconductor substrates of Si, GaAs, and GaP. Characterization of crystallization kinetics, crystallization mechanism, and film/substrate interdiffusion at temperatures near the glass-transition temperature by structural, calorimetric, and electrical measurements. Examination of structural relaxation by electrical resistivity measurements during post-deposition annealing. Measurement of diffusion and interdiffusion by a combination of Rutherford back scattering and Auger electron spectroscopy techniques. Assessment of reactions involving crystallization and possible phase separation, involving TEM analysis of in situ annealing, and supplementary SEM and X-ray diffraction measurements.
511. THERMODYNAMICS AND KINETICS OF PHASE FORMATION OF THIN-FILM METAL ON GALLIUM ARSENIDE

Y. A. Chang  
Dept. of Metallurgical and Mineral Engineering  
Phone: (608) 263-1821  
M. G. Lagally  
Dept. of Metallurgical and Mineral Engineering  
Phone: (608) 263-1821  
$122,680 01-3

Investigate the thermodynamics and kinetics of phase formation for metal films deposited on GaAs. Investigation consists of (1) bulk phase equilibrium and thermodynamic determinations of selected Ga-As-M ternaries and the associated thermodynamic modeling and phase diagram calculations; (2) bulk diffusion-couple measurements of GaAs-M; and (3) lateral thin-film diffusion couple measurements of GaAs-M and thin-film studies of M on GaAs and of GaAs on M. Systems under investigation are Ga-As-Os, Ga-As-Pd, and Ga-As-W. Phase equilibrium determinations using X-ray diffraction, metallography, microprobe, differential thermal analysis (DTA) and differential scanning calorimetry (DSC). Thermodynamic properties for Ga-M compound phases measured using a solid-state emf method. Diffusion paths in GaAs-M determined by means of microprobe analysis with bulk diffusion couples. The thin-film lateral diffusion couples characterized primarily by electron microscopy. Reactions and phase formation in thin films of metal on GaAs and of GaAs on metal characterized by electron microscopy and a variety of thin-film compositional, microstructural, and crystallographic analysis.

512. OPTICAL STUDIES OF DYNAMICAL PROCESSES IN DISORDERED MATERIALS

W. M. Yen  
Dept. of Physics  
Phone: (608) 263-7475  
$119,002 02-2

Comprehensive and detailed study of relaxation and energy transfer in and among optically excited states in disordered or amorphous systems and in certain ceramics. Application of new spectroscopic techniques to provide more fundamental understanding of prototypical transport processes, e.g. in rare earth-doped glasses or in mullites containing variable size crystallites. Advanced laser techniques, fluorescence line narrowing (FLN) and time-resolved FLN, measurement of coherent optical transients, photoacoustic and photocaloric methods, far infrared study using a free electron laser. Measurement and analysis of linewidths and lineshapes and of their temperature dependence, testing of models for the underlying mechanisms (e.g., ion-phonon interactions, two-level system model).
513. ANALYSIS OF MICROPHASE SEPARATION IN ION CONTAINING POLYMERS

S. L. Cooper
Dept. of Chemical Engineering
Phone: (508) 262-1092

$233,050 (24 Months) 03-1

Investigations of the microstructure of several ionomer systems using techniques which probe different aspects of the structure. Development of a unified model of the morphology which can rationalize the unique physical properties of these materials. Of special interest, the Nafion® ionomers because of their applications in electrochemical processes as selectively permeable membranes. The local arrangement of atoms in the ionic domains studied using Extended X-ray Absorption Fine Structure (EXAFS) analysis and XANES spectroscopy. Information about larger scale structure obtained from X-ray scattering and transmission electron microscopy experiments. To better understand the reason for differences between various ion containing polymers, the effects of several composition and preparation variables explored.

514. SURFACE EXCITATIONS AND THEIR INTERACTION WITH LOW ENERGY ELECTRONS

S. Y. Tong
Dept. of Physics and Surface Studies Laboratory
Phone: (414) 963-4474

$90,428 02-3

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

Small Business Innovation Research
PHASE I SBIR PROJECTS

The goal of the Phase I projects is to determine the technical feasibility of the ideas proposed.

CERAMATEC, INC.
163 West 1700 South
Salt Lake City, UT 84115

550. HIGH THERMAL CONDUCTIVITY DISPERSION-STRENGTHENED SILICON NITRIDE

D. W. Richerson
Phone: (801) 486-5071

$49,848 (6 months) SBIR

Phase I will concentrate on evaluating the effects of adding 20 through 50% SiC particles and whiskers to Si_3N_4 starting materials and the effects of using alpha versus beta SiC. Baseline evaluation will include density, flexure strength, fracture toughness (K_{IC}), hardness and microstructure. Selected specimens will be further evaluated by thermal conductivity measurements and by actual testing as cutting tool inserts. Directions for optimization will be identified for study in Phase II.

FLOW RESEARCH COMPANY
21414 68th Ave. S.
Kent, WA 98032

551. CLUSTER BEAM TECHNOLOGY FOR THIN FILMS

A. C. Day
Phone: (206) 872-7080

$49,826 (6 months) SBIR

A systematic investigation of the Ionized Cluster Beam (ICB) deposition technique. Research will address the following: (1) how clusters are formed; (2) what the actual makeup is of a cluster beam; (3) how clusters and other beam species interact to form thin films; and (4) what intrinsic advantages ICB holds over other techniques. The Phase I approach will combine modeling and experimental work with an emphasis on front-end issues of beam generation and characterization. A limited series of thin films will also be grown and studied.
552. DEVELOPMENT OF HIGH-TEMPERATURE AMORPHOUS ALLOYS

R. Wang
Phone: (206) 872-7080

$ 49,845 (6 months) SBIR

Development of high-temperature amorphous intermetallic alloys with crystallization temperatures, $T_x$, as high as $1000^\circ C$ ($1273^\circ K$) for extended application in oxidation, sulfidation, corrosion, wear, and catalytic reactions. Phase I will establish criteria for quantitative interpretation and prediction of the crystallization temperature of binary amorphous intermetallic compounds and will develop two amorphous alloys designed to reach high thermal stability.

553. PROCESSING SCIENCE: UNDERSTANDING AND CONTROL OF THE WHISKER MATRIX INTERFACE IN CERAMIC-CERAMIC COMPOSITES

B. Sonupariak
Phone: (206) 872-7080

$ 49,964 (6 months) SBIR

This work will evaluate the feasibility of using processing science to tailor the composition and interface bonding of whisker-reinforced ceramic composites. Microstructural control will be evaluated by varying gel structures (colloidal versus polymeric) and sintering (liquid state versus solid state) conditions. The mullite-mullite and mullite-alumina composites were selected for the study of matrix-fiber interfaces because they provide the optimum characteristics for development of a model system. Work is planned to investigate the effects of microstructure and interface reactions on the fracture toughness and strength.
554. MECHANICAL RELIABILITY OF SUPERPlASTICALLY FORGED SILICON NITRIDE

P. C. Panda
Phone: (607) 257-4514

$50,000 (6 months) SBIR

This project will investigate whether forging improves the reliability of silicon nitride components. Phase I research will carry out a full-length statistical study and measure the Weibull modulus for superplastically forged silicon nitride.

555. SURFACE FIGURE MEASUREMENTS OF X-RAY OPTICS

T. C. Bristow
Phone: (716) 385-6760

$49,867 (6 months) SBIR

This project will study the measurement of surface figure of X-ray mirrors and optical components. The proposed measurement technique will not contact the surface of the mirror and will be capable of a measurement during the polishing cycle. The technique also can measure a low-reflectance or uncoated surface. The effects of noise, focusing errors, and vibration will be studied for a stationary optic located on a polishing machine.
PHYSICAL OPTICS CORPORATION
3306 Dow Ave.
Redondo Beach, CA 90278

556. UV HOLOGRAPHIC MIRRORS WITH HIGH DIFFRACTION EFFICIENCY

J. Hannson
Phone: (213) 371-3909

$ 49,336 (6 months) SBIR

A new holographic approach is proposed for production of UV optical elements, which is based on nonlinear holographic recording of second-harmonic Bragg structure. This fabrication technique of UV optics will have at least two orders of magnitude lower cost than the conventional vacuum deposition technology. The high reflectivity of the holographic rugate mirror is achieved by a very large number of layers (up to 1000) formed in a single holographic recording.

SYN CRYS, INC.
122 E. Division Road
Oak Ridge, TN 37830

557. A SEARCH FOR METAL OXIDE-METAL NITRIDE EUTECTIC SYSTEMS

G. W. Clark
Phone: (615) 482-3411

$ 30,953 (6 months) SBIR

The chemical stability and the tendency for eutectic solidification will be explored for specific periodic group III and IV metal oxide-metal nitride systems. Blended oxide-nitride powders will be pressed into pellets, heated on W, Mo, or Ta strip heaters to form melts and then solidified. Free energy of formation data will be used to estimate the regions of existence and the chemical stability of these systems. Oxygen and nitrogen partial pressures will be maintained over melts and during the solidification process to enhance the coexistence of the oxides and nitrides. The high-temperature stability and solidification morphology for the systems Al₂O₃-TiN, Y₂O₃-TiN, ZrO₂-TiN, Al₂O₃-ZrN, Y₂O₃-ZrN, and ZrO₂-ZrN will be studied.
Development of a strongly corrosion-resistant amorphous layer on the surface of 304 stainless steel by the use of high-energy MeV ion beam processing. The best combination of ion parameters such as mass, energy, dose, and specific elemental addition for obtaining an amorphous layer will be determined. The aqueous corrosion behavior of the coated stainless steel will be investigated by standard electrochemical tests. The microstructural characterization and the corrosion kinetics will be studied by more advanced surface and electrochemical techniques.
PHASE II SBIR PROJECTS

The Phase II projects are a continuation of the successful Phase I projects. The goal of the Phase II projects is to determine commercial feasibility.

ADELPHI TECHNOLOGY
13800 Skyline Blvd.
Woodside, CA 94062

559. THE CONSTRUCTION OF A SOFT X-RAY SOURCE USING TRANSITION RADIATION FOR LITHOGRAPHY

M. A. Piestrup
President
Phone: (415) 851-0633

$478,564 (24 months) SBIR

Development of transition radiators with high average photon flux for X-ray sources. Investigation of the use of these sources for X-ray lithography in the production of integrated circuits. Measurement of total photon flux from several foil stacks using a newly developed high-average-current, 50 Mev accelerator. The radiators will be tested at full beam current for maximum flux and target lifetime.

ANALYSIS CONSULTANTS
21831 Zuni Drive
El Toro, CA 92630

560. THE DESIGN AND FABRICATION OF FLAT PANELS WITH HIGH ACOUSTIC TRANSMISSIVITY

B. G. Martin
President
Phone: (714) 380-1204

$490,000 (24 months) SBIR

Feasibility of constructing media with high acoustic transmissivity for all frequencies. Program objectives are to determine theoretically the acoustic velocity profile which gives maximum transmissivity, to design flat test panels based on the theoretical results, and to fabricate test panels and measure the transmissivity vs. frequency from 0.5 MHz to 5MHz.
Eddy current nondestructive evaluation techniques to characterize melt depth and to detect flaws in laser glazed metallic surfaces. Principal Phase I findings include a correlation between blazed depth and eddy current impedance plane phase angle, flaw detection using split core differential probe designs, and temperature effect characterization during on-line processing. Phase II objectives include an extension of eddy current/material interaction theory, development of high temperature eddy current probe systems, design of rapid scanning laser glazing apparatus, establishment of signal processing techniques, finite element modeling, and the design, test, and optimization of a laser glazing prototype system. Findings will be incorporated in a closed loop laser processing system having multi-variable control based on eddy current NDE sensor technology.

Liquid phase sintering of SiCA1ON ceramics, with improved processing and compositional control, to yield ceramics with smaller critical flaws and higher strengths. Investigation of physical properties as a function of Al2O3 content to demonstrate the ceramic engineering possible with SiCA12O3. Novel sintering techniques to show economical densification of SiCA1ON ceramics. Elevated temperature strength and creep measurements to determine the temperature range where liquid phase sintered SiCA1ON can be applied. Investigation of the stability of the solid solution in air, N2, and Ar at temperatures up to 1700°C.
C-8

CERAMATEC INC.
163 West 1700 South
Salt Lake City, UT 84115

562. FABRICATION AND CHARACTERIZATION OF CERAMIC MATRIX-CERAMIC WHISKER COMPOSITES WITH RANDOM ORIENTATION OF THE WHISKERS

L. Viswanathan
Senior Research Scientist
Phone: (801) 486-5071

$498,816 (24 months) SBIR

Fabrication and characterization of ceramic matrix-SiC whisker composites by pressureless sintering for advanced heat engines. Development of powder processing methods that yield randomly oriented whisks. The materials to be studied are Al₂O₃ + SiC and Si-Al₂O₃ + SiC. The former is expected to retain toughness in excess of 8MPa (m)¹/² in excess of 1000°C and the latter to 1300°C.

CERAMIC FINISHING COMPANY
P. O. Box 498
State College, PA 16804

564. FRACTURE MECHANICS INVESTIGATION OF GRINDING OF CERAMICS

Henry P. Kirchner
President
Phone: (814) 238-4270

$107,988 (24 months) SBIR

Application of contact fracture mechanics to investigate mechanisms of material removal and damage penetration during abrasive machining of ceramics. Phase I research investigated the mechanisms of material removal including crushing by mixed mode fracture ahead of the diamond point and chipping at lateral cracks propagating in response to residual stresses induced by elastic relaxation against the irreversibly deformed zone on unloading. The objective: determine the relative importance of crushing ahead of the diamond point and chipping alongside the track as a result of lateral cracking, for various material properties and grinding conditions, investigate the role of crushing in reducing the residual stresses that are responsible for lateral cracking, develop mathematical models by adapting available models for static indentations. The experimental results will be compared with results predicted by these models.
565. HORIZONTAL GROWTH OF SILICON SHEET CRYSTALS VIA EDGE-SUPPORTED PULLING (ESP) FROM MELT CONTAINED IN A COLD CRUCIBLE

Joseph F. Wenckus
President
Phone: (617) 899-5522

$142,509 SBIR

Explore the feasibility of growing silicon sheet crystals horizontally using the edge-supported pulling (ESP) process from silicon melts contained in an RF heated crucible. The vertical ESP process provides exceptionally stable sheet growth conditions, but sheet growth rates achieved to date are severely restricted by the rate of heat dissipation from the narrow sheet/melt interface. This program endeavors to integrate the unique operational features of the cold crucible with the equally unique attributes of the ESP process to demonstrate the feasibility of the horizontal edge-supported pulling method for the production of silicon crystals.

566. MATHEMATICAL MODELING OF ELECTROCHEMISTRY OF STRESS CORROSION CRACKING

T. R. Beck
Phone: (206) 632-5965

$164,149 (18 months) SBIR

Mathematical modeling of the electrochemical transport and kinetic processes that occur in tunnel corrosion of aluminum, correlative experiments on salt film properties using the shielded electrode technique, relation of the above to stress corrosion cracking.
567. DEVELOPMENT OF ND-FE-B METAL-MATRIX MAGNETS

Reinhold M. W. Strnat
Research Engineer
Phone: (513) 299-0313, 2717

Heat-bonded composites of hard magnetic alloy powders in a ductile metal matrix fabricated and characterized for potential high energy permanent magnet applications. Refinement of techniques of comminuting, aligning, pressing, and bonding to produce good physical compacts that also have optimized magnetic properties. To prevent corrosion, grinding under protective gas and liquid will be tried with emphasis on minimizing the production of very fine particles. Methods to coat powders with elements like Zn, Sn, and Cu will be investigated. Modified magnetic materials such as Co- and Dy-containing Nd-Fe-B will be studied. Measurement of short-term reversible and long-term irreversible flux losses, long-term elevated temperature stability of magnetic flux, coercivity, and hysteresis loop shape. SEM and optical microscopy to characterize the bond between matrix and metal and magnetic constituent after aging.

568. THE DIRECT PRODUCTION OF INTERMETALLIC COMPOUND POWDER

J. C. Withers
Technical Manager
Phone: (602) 749-3257

Examination of the feasibility of producing nickel and titanium aluminide intermetallic alloy powder by the direct reduction of metal chloride precursors. Definition of optimal operating conditions for producing Ni₃Al microalloyed with boron with and without hafnium and with uniform inter and intraparticle composition in a particle size useful in current powder-metallurgy processing. A continuous quartz reactor will be designed and operated for the purpose of establishing technical feasibility. The technical issues are to determine thermodynamically the most favorable operating conditions for phase control and material balance, to determine experimentally the optimum operating parameters for enhancing the nucleation of alloyed particles, to establish the need for microscopic mixing of product, and to develop an empirical model to describe nucleation kinetics.
SUPERCON INC.
9 Eric Drive
Natick, MA  01760

569. INVESTIGATION TO DETERMINE THE COMMERCIAL FEASIBILITY OF IN SITU CU-NB COMPOSITES FOR HIGH STRENGTH, HIGH CONDUCTIVITY APPLICATION

J. Wong
Phone: (617) 655-0500

$116,667 (24 months) SBIR

Development of a procedure for determining the commercial feasibility of fabricating 'in situ' Cu-Nb multifilamentary composites for high stress, high conductivity applications. Maintenance of a low volume fraction of Nb to retain desirable electrical and thermal properties of Cu. Evaluation of composite formability, tensile and fatigue strengths, and electrical conductivity.
SECTION D

Major User Facilities
(Large Capital Investment)
The National Synchrotron Light Source (NSLS) facility consists of a 750 MeV storage ring for VUV and IR research and a 2.5 GeV storage ring for X-ray research. Attractive features of synchrotron radiation include high brightness and intensity, broad and continuous spectral range, high polarization and pulsed time structure (subnanosecond pulses). Since each of the 28 X-ray and 16 VUV beam ports can be split into from 2 to 4 beam lines, as many as 100 experiments could run simultaneously at the NSLS. A 6 pole superconducting wiggler magnet and a 38 period permanent magnet undulator have been constructed, and several wiggler and undulator magnets are being designed which will significantly increase the photon intensity and brightness.

At NSLS a wide range of techniques are being used by solid state physicists, metallurgists, biologists, chemists, and engineers for basic and applied studies. Among the techniques are EXAFS (extended X-ray absorption fine structure), scattering, diffraction, topography, radiography, fluorescence, interferometry, gas phase spectroscopy, photoemission, radiometry, lithography, microscopy, dichroism, and infrared vibrational spectroscopy.

USER MODE

The policy for use of the NSLS is designed to enable the scientific community to cooperate in the design and fabrication of experimental apparatus. In addition to the beam lines constructed by the NSLS staff for general usage, a large number of beam lines have been designed and instrumented by "Participating Research Teams" (PRTs). The PRTs are given priority for up to 75% of their beam line(s) operational time for a three-year term. Research groups are now forming insertion device teams (IDTs) to design and instrument beam lines and insertion devices.

General Users can perform experiments on an NSLS facility beam line or on a PRT beam line which, after an initial commissioning period, are available for use by non-PRT members for at least 25% of its total operational time. In the latter case, PRTs will provide liaison and utilization support to General Users.

Proprietary research can be performed at the NSLS. A full-cost recovery fee is charged for the amount of beam time used. The DOE has granted the NSLS a Class Waiver, under the terms of which Proprietary Users of the NSLS will have the option to retain title to inventions that result from research performed at the NSLS.

Limited funding is available to scientists from U.S. institutions of higher education under the NSLS-HFBR Faculty/Student Support Program. The program is designed to defray expenses incurred by faculty/student research groups performing experiments at the NSLS or at the HFBR. It is aimed at university users having only limited grant support for their research and will be used to support only the most deserving cases.

PERSONS TO CONTACT FOR INFORMATION

Susan White-DePace (516) 282-7114
NSLS Department, Building 725B (FTS) 666-7114
Brookhaven National Laboratory
## NATIONAL SYNCHROTRON LIGHT SOURCE

### TECHNICAL DATA

<table>
<thead>
<tr>
<th>Facilities</th>
<th>Key Features</th>
<th>Operating Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>VUV electron storage ring</td>
<td>high brightness, continuous wavelength range (&gt; 5Å) 16 beam ports.</td>
<td>0.75 GeV electron energy</td>
</tr>
<tr>
<td>X-ray electron storage ring</td>
<td>high brightness, continuous wavelength range ( &gt; .5Å) 28 beam ports</td>
<td>2.5 GeV electron energy</td>
</tr>
</tbody>
</table>

### Instruments

#### Monochromators:
- **plane grating**: $12\AA < \lambda < 1500\AA$; high resolution
- **zone plate**: $8\AA < \lambda < 100\AA$; moderate resolution
- **toroidal grating**: $10\AA < \lambda < 2500\AA$; high intensity, moderate and high resolution
- **extended range grasshopper**: $10\AA < \lambda < 2000\AA$; high resolution
- **Wadsworth**: $300\AA < \lambda < 3000\AA$; high intensity, moderate resolution
- **Seya&Czerny Turner**: $1200\AA < \lambda < 12000\AA$; high intensity, moderate resolution
- **two crystal**: $0.04\AA < \lambda < 2500\AA$; high resolution, fixed exit beam
- **two crystal/two grating**: $2.5\AA < \lambda < 2500\AA$; high resolution, fixed exit beam

#### Six circle spectrometer/diffractometers:
- high positional and rotational accuracy

#### Experimental stations:
- photoemission, magnetic circular dichroism, fluorescence, gas phase spectroscopy, microscopy, lithography, holography, EXAFS, inelastic scattering, crystallography, radiometry, topography, small angle scattering

#### Permanent magnet undulator
- $30\AA < \lambda < 5000\AA$; high intensity and brightness
The Brookhaven High Flux Beam Reactor (HFBR) operates at a power of 60 megawatts and provides an intense source of thermal neutrons (total thermal flux = $1.0 \times 10^{15}$ neutrons/cm²-sec). The HFBR was designed to provide particularly pure beams of thermal neutrons, uncontaminated by fast neutrons and by gamma rays. A cold source (liquid hydrogen moderator) provides enhanced flux at long wavelengths ($> 4 \, \AA$). A polarized beam spectrometer, triple-axis spectrometers and small-angle scattering facilities are among the available instruments. Special equipment for experiments at high and low temperatures, high magnetic fields, and high pressure is also available. The emphasis of the research efforts at the HFBR has been on the study of fundamental problems in the fields of solid state and nuclear physics and in structural chemistry and biology.

**USER MODE**

Experiments are selected on the basis of scientific merit by a Program Advisory Committee (PAC), composed of the specialists in relevant disciplines from both within and outside BNL. Use of the facilities is divided between Participating Research Teams (PRT's) and general users. PRT's consist of scientists from BNL or other government laboratories, universities, and industrial labs who have a common interest in developing and using beam facilities at the HFBR. In return for their development and management of these facilities, each PRT is assigned up to 75% of the available beam time, with the remainder being reserved for general users. The PAC reviews the use of the facilities by the PRT's and general users and assigns priorities as required.

A limited amount of funding will be available to scientists from U.S. institutions of higher education under the NSLS-HFBR Faculty/Student Support Program. The program is designed to defray expenses incurred by faculty/student research groups performing experiments at the National Synchrotron Light Source or at the HFBR. It is aimed at university users having only limited grant support for their research, and will be used to support only the most deserving cases.

**PERSON TO CONTACT FOR INFORMATION**

D. Rorer (516) 282-4056
HFBR - Bldg. 750 FTS 666-4056
Brookhaven National Laboratory
## High Flux Beam Reactor

### Technical Data

<table>
<thead>
<tr>
<th>Instruments</th>
<th>Purpose and Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Solid State Physics</strong></td>
<td></td>
</tr>
<tr>
<td>4 Triple-axis Spectrometers</td>
<td>Inelastic scattering; diffuse scattering; powder diffractometer; polarized beam. Energy range: 2.5 MeV, ( &lt; E_0 &lt; 200 ) MeV, Q range: 0.03 ( &lt; Q &lt; 10 ) Å(^{-1})</td>
</tr>
<tr>
<td><strong>Biology</strong></td>
<td></td>
</tr>
<tr>
<td>Small Angle Neutron Scattering</td>
<td>Studies of large molecules. Located on cold source with 20 x 20 cm(^2) position-sensitive area detector. Sample detector distance (&lt; 2 ) meter. Incident wavelength 4 Å (&lt; \lambda_0 &lt; 10 ) Å</td>
</tr>
<tr>
<td>Diffractometer</td>
<td>Protein crystallography 20 x 20 cm(^2) area detector ( \lambda_0 = 1.57 ) Å</td>
</tr>
<tr>
<td><strong>Chemistry</strong></td>
<td></td>
</tr>
<tr>
<td>2 Diffractometers</td>
<td>Single-crystal elastic scattering 4-circle goniometer ( 1.69 ) Å (&lt; \lambda_0 &lt; 0.65 ) Å</td>
</tr>
<tr>
<td>1 Triple-axis Spectrometer</td>
<td>Inelastic scattering Diffuse scattering Powder diffractometry</td>
</tr>
<tr>
<td><strong>Nuclear Physics</strong></td>
<td></td>
</tr>
<tr>
<td>3 Spectrometers</td>
<td>Neutron capture studies Energy range: 0.025 eV (&lt; E_0 &lt; 25 ) KeV</td>
</tr>
<tr>
<td>TRISTAN II (Isotope Separator)</td>
<td>Spectroscopic study of neutron-rich unstable isotopes produced from U-235 fission</td>
</tr>
<tr>
<td><strong>Irradiation Facilities</strong></td>
<td></td>
</tr>
<tr>
<td>7 Vertical Thimbles</td>
<td>Neutron activation; production of isotopes; thermal flux: 8.3 ( \times 10^{14} ) neutrons/cm(^2)-sec; fast ( (&gt;0.5 ) MeV) flux: 3 ( \times 10^{14} ) neutrons/cm(^2)-sec.</td>
</tr>
</tbody>
</table>
The neutron scattering facilities at the High Flux Isotope Reactor (HFIR) are used for long-range basic research on the structure and dynamics of condensed matter. Active programs exist on the magnetic properties of matter, lattice dynamics, defect-phonon interactions, fluxoid lattices in superconductors, liquid structures, and crystal structures. The HFIR is a 100-MW, light-water moderated reactor with an unsurpassed record of operating time (better than 90%). The central flux is $5 \times 10^{15}$ neutrons/cm$^2$-sec, and the flux at the inner end of the beam tubes is slightly greater than $10^{15}$ neutrons/cm$^2$-sec. A wide variety of neutron scattering instruments have been constructed with the support of the Division of Materials Sciences. Three of these are unique within this country: the double-crystal small-angle diffractometer, the correlation chopper, and the wide-angle time-slicing diffractometer.

USER MODE

These facilities are open for use by outside scientists on problems of high scientific merit. Written proposals are reviewed for scientific feasibility by an external review committee. It is expected that all accepted experiments will be scheduled within six months of the receipt of the proposal. No charges for the use of the beams will be assessed for research to be published in the open literature. The cost of extensive use of ORNL shop or computer facilities must be borne by the user. Financial assistance is available for the travel and living expenses of users from U.S. universities. Inexperienced users will normally collaborate with an ORNL staff member. Proprietary experiments can be carried out after a contract has been arranged based on full cost recovery, including a charge for beam time. A brochure describing the facilities and a booklet giving user procedures is available on request.

PERSON TO CONTACT FOR INFORMATION

R. M. Nicklow
Solid State Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

(615) 574-5240
FTS 624-5240
# Technical Data

<table>
<thead>
<tr>
<th>Beam No.</th>
<th>Instrument</th>
<th>Operating Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>HB-1</strong></td>
<td>Triple-axis polarized-beam</td>
<td>Beam size - 2.5 by 3 cm max Flux - $2.6 \times 10^6$ neut/cm$^2$ s at sample (polarized) Vertical magnetic fields to 5 T Horizontal fields to 2 T Variable $E_0$</td>
</tr>
<tr>
<td><strong>HB-1A</strong></td>
<td>Triple-axis, fixed $E_0$</td>
<td>$E_0 = 14.7$ MeV, 2.353 angstroms Beam size - 5 by 3.7 cm max Flux - $9 \times 10^6$ neut/cm$^2$ s at sample with 40 ft collimation</td>
</tr>
<tr>
<td><strong>HB-2A</strong></td>
<td>Liquid diffractometer with linear position sensitive detector</td>
<td>Beam size - 1 by 3.4 cm max Detector covers 130° scattering angle; Wavelength = 0.89 angstrom Flux - $6.8 \times 10^5$ neut/cm$^2$ s at sample with 20 min collimation</td>
</tr>
<tr>
<td><strong>HB-2, HB-3</strong></td>
<td>Triple-axis, variable $E_0$</td>
<td>Beam size - 5 by 3.7 cm max Flux - $10^7$ neut/cm$^2$ s at sample with 40 min collimation</td>
</tr>
<tr>
<td><strong>HB-3A</strong></td>
<td>Double-crystal small-angle diffractometer</td>
<td>Beam size - 4 x 2 cm max Flux - $10^5$ neut/cm$^2$ s Wavelength = 2.6 angstroms Resolution - $4 \times 10^{-5}$ angstroms$^{-1}$</td>
</tr>
<tr>
<td><strong>HB-4A</strong></td>
<td>Four-circle diffractometer</td>
<td>Beam size - 5 x 5 mm Flux - $2 \times 10^6$ neut/cm$^2$ s with 9 min collimation Wavelength = 1.015 angstrom</td>
</tr>
<tr>
<td><strong>Wide-angle time-slicing diffractometer</strong></td>
<td></td>
<td>Beam size - 2 x 3.7 cm max Flux - $2 \times 10^6$ neut/cm$^2$ s with 9 min collimation Wavelength = 1.015 angstrom Curved linear position sensitive detector covering 130°</td>
</tr>
<tr>
<td><strong>HB-4</strong></td>
<td>Correlation chopper</td>
<td>Beam size - 5 x 3.7 cm Flight path - 1.5 m 70 detectors covering 130° Variable $E_0$ Variable pulse width</td>
</tr>
</tbody>
</table>
INTENSE PULSED NEUTRON SOURCE

Argonne National Laboratory
Argonne, Illinois 60439

IPNS is an intermediate level pulsed spallation source dedicated to research on condensed matter. The peak thermal flux is about $3 \times 10^{14}$ n/cm$^2$ sec. The source has some unique characteristics that promise to open up new scientific opportunities:

- high fluxes of epithermal neutrons (0.1-10 eV)
- pulsed nature, suitable for real-time studies and measurements under extreme environment

Two principal types of scientific activity are underway at IPNS: neutron diffraction, concerned with the structural arrangement of atoms (and sometimes magnetic moments) in a material and the relation of this arrangement to its physical and chemical properties, and inelastic neutron scattering, concerned with processes where the neutron exchanges energy and momentum with the system under study and thus probes the dynamics of the system at a microscopic level. At the same time, it is expected that the facilities will be used for fundamental physics measurements as well as for technological applications, such as stress distribution in materials and characterization of zeolites, ceramics, and hydrocarbons.

USER MODE

IPNS is available without charge to qualified scientists doing fundamental research. Selection of experiments is made on the basis of scientific merit by a Program Committee consisting of eminent scientists, mostly from outside Argonne. Scientific proposals (2 pages long) are submitted twice a year and judged by the Program Committee. Full details, including a User's Handbook, Proposal and Experimental Report Forms, can be obtained from the Scientific Secretary, Dr. T. G. Worlton, IPNS, Building 360, Argonne National Laboratory.

PERSONS TO CONTACT FOR INFORMATION

B. S. Brown, Acting Division Director (312) 972-4999
FTS 972-4999

T. G. Worlton, Scientific Secretary (312) 972-8755
FTS 972-8755

Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439
## NEUTRON SCATTERING

<table>
<thead>
<tr>
<th>Facility (Instrument Scientist)</th>
<th>Assignment</th>
<th>Range Wave-vector Å⁻¹</th>
<th>Wave-vector Energy</th>
<th>Resolution Wave-vector Å⁻¹</th>
<th>Resolution Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Special Environment Powder Diffractometer (J. D. Jorgensen)</td>
<td>F5</td>
<td>0.5-50 Å⁻¹</td>
<td>*</td>
<td>0.35%</td>
<td>*</td>
</tr>
<tr>
<td>General Purpose Powder Diffractometer (J. Faber, Jr., R. Hitterman)</td>
<td>F2</td>
<td>0.5-100 Å⁻¹</td>
<td>*</td>
<td>0.25%</td>
<td>*</td>
</tr>
<tr>
<td>Single Crystal Diffractometer (A. J. Schultz)</td>
<td>F6</td>
<td>2-20 Å⁻¹</td>
<td>*</td>
<td>2%</td>
<td>*</td>
</tr>
<tr>
<td>Low-Resolution Medium-Energy Chopper Spectrometer (C.-K. Loong)</td>
<td>F4</td>
<td>0.1-30 Å⁻¹</td>
<td>0-0.6 ev</td>
<td>0.02 k₀</td>
<td>0.05 E₀</td>
</tr>
<tr>
<td>High-Resolution Medium-Energy Chopper Spectrometer (D. L. Price)</td>
<td>H3</td>
<td>0.3-9 Å⁻¹</td>
<td>0.0-0.4 eV</td>
<td>0.01 K₀</td>
<td>0.02 E₀</td>
</tr>
<tr>
<td>Small-Angle Scattering Diffractometer (J. E. Epperson, P. Thiyagarajan)</td>
<td>C1</td>
<td>0.006-0.3 Å⁻¹</td>
<td>*</td>
<td>0.004 Å⁻¹</td>
<td>*</td>
</tr>
</tbody>
</table>

* No energy analysis

Wave-vector, \( K = 4\pi \frac{\sin \theta}{\lambda} \)

### NEUTRON BEAMS FOR SPECIAL EXPERIMENTS

<table>
<thead>
<tr>
<th>Beam Tube</th>
<th>Current Use</th>
<th>Flight Path Length (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>F3</td>
<td>eV Spectrometer</td>
<td>10</td>
</tr>
<tr>
<td>C2</td>
<td>Polarized Neutron Exp.</td>
<td>10</td>
</tr>
<tr>
<td>F1</td>
<td>n(P) Spectrometer</td>
<td>13.6</td>
</tr>
<tr>
<td>H1</td>
<td>Glass Diffractometer</td>
<td>10</td>
</tr>
<tr>
<td>H2</td>
<td>QENS Spectrometer</td>
<td>8</td>
</tr>
</tbody>
</table>
The Los Alamos Neutron Scattering Center (LANSCE) facility is a pulsed spallation neutron source driven by the 800 MeV Los Alamos Meson Physics Facility (LAMPF) linear accelerator. Neutron scattering research is being carried out at LANSCE on six time-of-flight spectrometers. These are as follows: 1) a 32-m neutron powder diffractometer; 2) a single crystal diffractometer based on the Laue-TOF technique; 3) a filter difference spectrometer for chemical and optic mode spectroscopy; 4) a constant-Q spectrometer for studies of elementary excitations in single crystals; 5) a high intensity powder diffractometer, and 6) a low-Q diffractometer for small angle scattering studies which is located at a liquid hydrogen cold neutron source. A considerable effort is directed toward pulsed source instrument development including a chopper spectrometer, a neutron Anger camera and a back-scattering spectrometer for quasielastic scattering. The Proton Storage Ring (PSR) has reached 30% of its design intensity and will shortly enable LANSCE to deliver neutron pulses with the highest peak thermal flux for neutron scattering research in solid state physics, chemistry, biology and materials science.

USER MODE

During the initial start up of the PSR, LANSCE will operate in a collaborative mode. To propose an experiment, contact J. Eckert or the scientist responsible for the appropriate instrument. When the LANSCE facility is completed, it will be operated as a national user facility with formal proposals for experiments reviewed by a Program Advisory Committee (PAC) to allocate two-thirds of the available beam time. The PAC will evaluate proposals on the basis of scientific excellence and optimal use of LANSCE capabilities. One-third of the neutron scattering beam time is reserved for Laboratory discretionary research, research pertinent to DOE applied program goals, and instrument development. The LANSCE instrumentation is available without charge for nonproprietary research. The facility is open to all U.S. citizens and permanent resident aliens and to visits of less than seven working days for citizens of nonsensitive countries. DOE approval is required for any other foreign national visits.

PERSON TO CONTACT FOR INFORMATION

Juergen Eckert
MS H805, Group P-8
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

(505) 667-6069 or
(FTS) 843-6069
Proton Source | LAMPF + PSR
---|---
Proton Source Current | 1000 A
Proton Source Energy | 800 MeV
LANSCE Proton Current | 100 A
Proton Pulse Width | 0.27 s
Repetition Rate | 12 Hz
Epithermal Neutron Current (n/eV.Sr.S) | $3.2 \times 10^{12}/E$
Peak Thermal Flux (n/cm².S) | $1.7 \times 10^{16}$

**INSTRUMENTS**

32-m Neutron Powder Diffractometer (J. Goldstone, Responsible)
- Powder diffraction
- Wave vector 0.3-50 Å⁻¹
- Resolution 0.15%

Single Crystal Diffractometer (P. Vergamini, Responsible)
- Laue time-of-flight diffractometer
- Wave vectors 1-15 Å⁻¹
- Resolution 2% typical

Filter Difference Spectrometer (J. Eckert, Responsible)
- Inelastic neutron scattering, vibrational spectroscopy
- Energy trans. 15-600 meV
- Resolution 5-7%

High Intensity Powder Diffractometer (A. Williams, Responsible)
- Powder diffraction .7% resolution; liquids and amorphous materials diffraction 2% resolution

Constant-Q Spectrometer (R. Robinson, Responsible)
- Elementary excitations in single crystal samples
- Energy resolution 1-3%

Low Q Diffractometer (P. A. Seeger, Responsible)
- Small angle scattering at a liquid hydrogen cold source
- Wave vectors 0.003-1.0 Å⁻¹
SSRL is a National Users' Research Laboratory for the application of synchrotron radiation to research in materials science, chemistry, biology, physics, engineering and medicine. In addition to scientific research utilizing synchrotron radiation the Laboratory program includes the development of advanced sources of synchrotron radiation (e.g., insertion devices for the enhancement of synchrotron radiation, new ring designs). SSRL presently has 20 experimental stations. The radiation on nine stations is enhanced by insertion devices providing the world's most intense X-ray sources, and brightest soft X-ray source.

Commissioned in 1985 was the first experimental station on the 16 GeV storage ring, PEP. This line provides the world's most brilliant continuous X-ray beam, and will serve as a research tool and development center for future high-brilliance beam line concepts.

The primary research activities at SSRL are:

- X-ray absorption, small and large angle scattering as well as topographic studies of atomic arrangements in complex materials systems, including surfaces, extremely dilute constituents, amorphous materials and biological materials.

- Soft X-ray and VUV photoemission and photoelectron diffraction studies of electronic states and atomic arrangements in condensed and gaseous matter.

- Non-invasive angiography. X-ray lithography and microscopy.

SSRL serves approximately 500 scientists from 110 institutions working on over 170 active proposals. A wide variety of experimental equipment is available for the user and there are no charges either for use of the beam or for the facility-owned support equipment. Proprietary research may be performed on a cost-recovery basis by special arrangement.

**USER MODE**

SSRL is a user-oriented facility which welcomes proposals for experiments from all qualified scientists. Access is gained through proposal submittal and peer review. In the course of a year approximately 70% of all active proposals receive beam time. An annual Activity Report is available on request. It includes progress reports on about 100 experiments plus descriptions of recent facility developments. The booklet "General Information and Proposal Guidelines" includes information on proposal submittal and experimental station characteristics.

**PERSON TO CONTACT FOR INFORMATION**

K. M. Cantwell
SSRL, Bin 69 PO Box 4349
STANFORD, CA 94305
(415) 854-3300 ext. 3191
(FTS) 461-9300 ext. 3191
CHARACTERISTICS OF SSRL EXPERIMENTAL STATIONS

SSRL presently has 20 experimental stations, 19 of which are located on SPEAR and one on PEP. Nine of these stations are based on insertion devices while the remainder use bending magnet radiation.

<table>
<thead>
<tr>
<th>Horizontal Angular Acceptance (Mrad)</th>
<th>Mirror Cutoff (KeV)</th>
<th>Monochromator</th>
<th>Energy Range (eV)</th>
<th>Resolution ΔE/E</th>
<th>Approximate Dedicated Spot Size (mm)</th>
<th>Instrumentation</th>
</tr>
</thead>
<tbody>
<tr>
<td>INSERTION DEVICE STATIONS</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>End Stations</strong></td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>IV-2 (8 pole)</td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Focused</td>
<td>4.6</td>
<td>10.2</td>
<td>Double Crystal</td>
<td>2800-21000</td>
<td>-5x10^-4</td>
<td>2.0 x 6.0</td>
</tr>
<tr>
<td>Unfocused</td>
<td>1.0</td>
<td>-</td>
<td>Double Crystal</td>
<td>2800-45000</td>
<td>-10^-4</td>
<td>2.0 x 20.0</td>
</tr>
<tr>
<td>VI-2 (54 pole)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Focused</td>
<td>2.3</td>
<td>22</td>
<td>Double Crystal</td>
<td>2800-21000</td>
<td>-5x10^-4</td>
<td>2.0 x 6.0</td>
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<tr>
<td>Unfocused</td>
<td>1.0</td>
<td>-</td>
<td>Double Crystal</td>
<td>2800-45000</td>
<td>-10^-4</td>
<td>2.0 x 20.0</td>
</tr>
<tr>
<td>VII-2 (8 pole)</td>
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<td></td>
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<td></td>
<td></td>
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</tr>
<tr>
<td>Focused</td>
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<td>10.2</td>
<td>Double Crystal</td>
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<td>1.0 x 6.0</td>
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<tr>
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<td>-</td>
<td>Double Crystal</td>
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<td>-10^-4</td>
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<tr>
<td><strong>Side Stations</strong></td>
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<tr>
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<td>-</td>
<td>Double Crystal</td>
<td>2800-45000</td>
<td>-5x10^-4</td>
<td>2.0 x 20.0</td>
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<tr>
<td>IV-3</td>
<td>1.0</td>
<td>-</td>
<td>Double Crystal</td>
<td>2800-45000</td>
<td>-10^-4</td>
<td>2.0 x 20.0</td>
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<tr>
<td>VII-1</td>
<td>1.0</td>
<td>-</td>
<td>Curved Crystal</td>
<td>6000-13000</td>
<td>-8x10^-4</td>
<td>0.6 x 3.0</td>
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<tr>
<td>VII-3</td>
<td>1.0</td>
<td>-</td>
<td>Double Crystal</td>
<td>2800-45000</td>
<td>-10^-4</td>
<td>2.0 x 20.0</td>
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<tr>
<td><strong>UNDULATOR LINES - VUV/SOFT X-RAY</strong></td>
<td></td>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>V-1</td>
<td>1.5</td>
<td>-</td>
<td>None</td>
<td>10-1200</td>
<td>27%</td>
<td>6.0 x 8.0</td>
</tr>
<tr>
<td><strong>UNDULATOR LINES - X-RAY</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>PEP 5B</td>
<td>Full</td>
<td>15.0</td>
<td>Double Crystal</td>
<td>12000-20000</td>
<td>-10^-6</td>
<td>0.6 x 6.0</td>
</tr>
<tr>
<td><strong>BENDING MAGNET LINES</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>X-RAY</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>I-4</td>
<td>2.2</td>
<td>-</td>
<td>Curved Crystal</td>
<td>6000-95000</td>
<td>-60 eV</td>
<td>0.25 x 0.5</td>
</tr>
<tr>
<td>I-5</td>
<td>1.0</td>
<td>-</td>
<td>Double Crystal</td>
<td>3800-29300</td>
<td>-10^-4</td>
<td>2.0 x 20.0</td>
</tr>
<tr>
<td>II-2 (focused)</td>
<td>4.8</td>
<td>8.9</td>
<td>Double Crystal</td>
<td>2800-8900</td>
<td>-5x10^-4</td>
<td>2.0 x 4.0</td>
</tr>
<tr>
<td>II-3</td>
<td>1.0</td>
<td>-</td>
<td>Double Crystal</td>
<td>2800-30000</td>
<td>-5x10^-4</td>
<td>2.0 x 20.0</td>
</tr>
<tr>
<td>II-4</td>
<td>1.0</td>
<td>-</td>
<td>None</td>
<td>3200-30000</td>
<td>4.0 x 15.0</td>
<td></td>
</tr>
<tr>
<td>Lifetimes Port</td>
<td>1.8</td>
<td>-</td>
<td>None</td>
<td>1-6</td>
<td>Bandpass &gt;10A</td>
<td>4.0 x .4</td>
</tr>
<tr>
<td><strong>VUV/SOFT X-RAY</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>I-1</td>
<td>2.0</td>
<td>-</td>
<td>Grasshopper</td>
<td>32-1000</td>
<td>Δλ = 1-.2A</td>
<td>2.0 x 1.0</td>
</tr>
<tr>
<td>I-2</td>
<td>4.0</td>
<td>-</td>
<td>Seya-Namioka</td>
<td>4-40</td>
<td>Δλ = 2-6A</td>
<td>1.0 x 3.0</td>
</tr>
<tr>
<td>III-1</td>
<td>2.0</td>
<td>-</td>
<td>Grasshopper</td>
<td>15-1200</td>
<td>Δλ = 0.05-2A</td>
<td>1.0 x 1.0</td>
</tr>
<tr>
<td>III-3</td>
<td>8-10</td>
<td>-</td>
<td>Jumbo</td>
<td>800-4000</td>
<td>0.35-7 eV</td>
<td>2.0 x 4.0</td>
</tr>
<tr>
<td>III-4</td>
<td>2.0</td>
<td>-</td>
<td>Multilayer</td>
<td>2-3000</td>
<td>White or</td>
<td>2.0 x 11</td>
</tr>
</tbody>
</table>

Specialized Portable Beam Line Instrumentation Available: VG Chamber, Perkin Elmer Chamber, CAD-4, SAS Camera
SECTION E

Other User Facilities
The National Center for Small-Angle Scattering Research (NCSASR) is supported by the National Science Foundation and the Department of Energy under an interagency agreement. The two main instruments available to users are the NSF-constructed 30-m small-angle neutron scattering facility (SANS) and the DOE-constructed 10-m small-angle X-ray scattering camera (SAXS). These instruments are intended to provide state-of-the-art capability for investigating structures of condensed matter on a global scale, e.g., from a few tens to several hundreds of angstroms. They are intended to serve the needs of scientists in the areas of biology, polymer science, chemistry, metallurgy and materials science, and solid state physics.

USER MODE

Beam time on these instruments is assigned, in general, on the basis of proposals submitted in advance. These are then reviewed by a panel of experts external to the Laboratory and are rated on the basis of scientific merit. When a favorable review has been received, a staff member of the NCSASR and the user agree, usually by telephone, on a time and duration for the experiment. Ordinary charges are borne by the Center, but extensive use of support facilities (shops, computing, etc.) must be paid by the user. Users may work in collaboration with one or more staff members if they wish, but such collaboration is not required. Proprietary experiments can be carried out after contractual agreement has been reached.

PERSONS TO CONTACT FOR INFORMATION

G. D. Wignall, SANS-NCSASR (615) 574-5237
Oak Ridge National Laboratory FTS 624-5237
Oak Ridge, Tennessee 37831

J. S. Lin, SAXS-NCSASR (615) 574-4534
Oak Ridge National Laboratory FTS 624-4534
Oak Ridge, Tennessee 37831

G. J. Bunick, SANS-NCSASR (615) 576-2685
Oak Ridge National Laboratory FTS 626-2685
Oak Ridge, Tennessee 37831

M. Gillespie, Secretary NCSASR (615) 574-5231
Oak Ridge National Laboratory FTS 624-5231
Oak Ridge, Tennessee 37831
E-2
NATIONAL CENTER FOR SMALL-ANGLE SCATTERING RESEARCH

Technical Data

30-m SANS Instrument Specifications

Monochromator: six pairs of pyrolytic graphite crystals
Incident wavelength: 4.75 angstroms or 2.38 angstroms
Wavelength resolution: delta lambda/lambda = 6%
Source-to-sample distance: 10 m
Beam size at specimen: 0.5-3.0 cm diam
Sample-to-detector distance: 1.5-18.5 m
K range: $5 \times 10^{-3} \leq K \leq 0.6$ angstroms$^{-1}$
Detector: 64 by 64 cm$^2$
Flux at specimen: $10^6$-$10^7$ neutrons/cm$^2$ s depending on slit sizes and wavelength

10-m SAXS Instrument Specifications

Monochromator: hot-pressed pyrolytic graphite
Incident wavelengths: 1.542 angstroms (CuK$\alpha$) or 0.707 angstroms (MoK$\alpha$)
Source-to-sample distances: 0.5, 1.0, 1.5, ..., 5.0 m
Beam size at specimen: 0.1 by 0.1 cm (fixed)
Sample-to-detector distances: 1, 1.5, 2.0, ..., 5 m
K range covered: $3 \times 10^{-3} \leq K \leq 0.3$ angstroms$^{-1}$ (CuK$\alpha$)
$6 \times 10^{-3} \leq K \leq 0.6$ angstroms$^{-1}$ (MoK$\alpha$)
Maximum flux at specimen: $10^6$ photons per second on sample-irradiated area 0.1 by 0.1 cm
Detector: 20- by 20-cm$^2$ (electronic resolution 0.1 by 0.1 cm$^2$)
Special features: deformation device for dynamic scattering experiments (time slicing in periods as short as 100 microseconds for oscillatory experiments or 10 s for transient relaxation experiments) and interactive graphics for data analysis
The Argonne National Laboratory Electron Microscopy Center for Materials Research provides unique facilities which combine the techniques of high-voltage electron microscopy, ion-beam modification, and ion-beam analysis, along with analytical electron microscopy.

The cornerstone of the Center is a High Voltage Electron Microscope (an improved Kratos/AEI EM7) with a maximum voltage of 1.2 MV. This HVEM is interfaced to two accelerators, a National Electrostatics 2 MV Tandem Ion Accelerator and a Texas Nuclear 300 kV ion accelerator, which can produce ion beams from 10 keV to 8 MeV of most stable elements in the periodic table. Procurement of a 600 kV injector is underway as a replacement for the 300 kV accelerator. These instruments together comprise the unique High-Voltage Electron Microscope-Tandem Accelerator Facility. The available ion beams can be transported into the HVEM to permit direct observation of the effects of ions and electrons on materials. In addition to the ion-beam interface, the HVEM has a number of specialized features (see following page), which allow for a wide range of in situ experiments on materials under a variety of conditions.

In addition to the HVEM-Tandem Facility, the Center's facilities include a JEOL 100 CXII transmission and scanning transmission electron microscope (TEM/STEM), equipped with an X-ray energy dispersive spectrometer (XEDS), and a Philips EM 420 TEM/STEM equipped with XEDS and an electron energy loss spectrometer (EELS). A Philips EM430 with an XEDS will be added shortly. Procurement of an advanced Analytical Electron Microscope (AEM) is underway. This state-of-the-art, field emission gun ultra-high vacuum AEM will operate up to 300 keV and have the highest available microanalytical resolution with capabilities for XEDS, EELS, and AES. As such, it will have substantially increased analytical capabilities for materials research over present-day instruments.

USER MODE

The Center is operated as a national resource for materials research. Qualified scientists wishing to conduct experiments using the HVEM/TANDEM facilities of the Center should submit a proposal to the person(s) named below. Experiments are approved by a Steering Committee following peer evaluation of the proposals. There are no use charges for basic research of documented interest to DOE. Use charges will be levied for proprietary investigations.

PERSON(S) TO CONTACT FOR INFORMATION

E. A. Ryan (312) 972-5222
and
H. Wiedersich (312) 972-5079
Electron Microscopy Center for Materials Research FTS 972-5222
Materials Science and Technology Division FTS 972-5079
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439
### Technical Data

#### Electron Microscopes

<table>
<thead>
<tr>
<th>High-Voltage Electron Microscope</th>
<th>Key Features</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Kratos/AEI EM7 (1.2 MeV)</strong></td>
<td>Resolution 3.5 Å lattice</td>
</tr>
<tr>
<td></td>
<td>Continuous voltage selection (100-1200 kv)</td>
</tr>
<tr>
<td></td>
<td>Current density 15 A/cm²</td>
</tr>
<tr>
<td></td>
<td>High-vacuum specimen chamber</td>
</tr>
<tr>
<td></td>
<td>Negative-ion trap</td>
</tr>
<tr>
<td></td>
<td>Electron and ion dosimetry systems</td>
</tr>
<tr>
<td></td>
<td>Video recording system</td>
</tr>
<tr>
<td></td>
<td>Ion-beam interface</td>
</tr>
<tr>
<td></td>
<td>Specimen stages 10 - 1300 K</td>
</tr>
<tr>
<td></td>
<td>Straining and environmental stages</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Transmission Electron Microscope</th>
<th>Key Features</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Philips EM 420 (120 keV)</strong></td>
<td>Resolution 2.0 Å lattice</td>
</tr>
<tr>
<td></td>
<td>Equipped with EELS, XEDS</td>
</tr>
<tr>
<td></td>
<td>Specimen stages 15 - 300 K</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Transmission Electron Microscope</th>
<th>Key Features</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>JEOL 100 CX (100 keV)</strong></td>
<td>Resolution 2.0 Å lattice</td>
</tr>
<tr>
<td></td>
<td>Equipped with STEM, XEDS</td>
</tr>
<tr>
<td></td>
<td>Specimen stages 300 - 900 K</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Analytical Electron Microscope</th>
<th>Key Features</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Being acquired (300 keV)</strong></td>
<td>State-of-the-art resolution</td>
</tr>
<tr>
<td></td>
<td>Ultra-high vacuum, Field Emission Gun</td>
</tr>
<tr>
<td></td>
<td>Equipped with EELS, XEDS, etc.</td>
</tr>
</tbody>
</table>

#### Accelerators

<table>
<thead>
<tr>
<th>Accelerator</th>
<th>Key Features</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>NEC Model 2 UDHS</strong></td>
<td>Terminal voltage 2 MV</td>
</tr>
<tr>
<td></td>
<td>Energy stability ±250 eV</td>
</tr>
<tr>
<td></td>
<td>Current density: H⁺, 10 μA/cm²</td>
</tr>
<tr>
<td></td>
<td>(typical) Ni⁺, 3 μA/cm²</td>
</tr>
</tbody>
</table>

| **Texas Nuclear 300-kV**         | Terminal voltage 300 kV |
|                                  | Energy stability ±300 eV |
|                                  | Current density: He⁺, 200 μA/cm² |
|                                  | (typical) Ni⁺, 2 μA/cm² |

| **NEC 600 kV Injector**          | Terminal voltage 600 kV |
|                                  | Energy stability ±60 eV |
|                                  | Current density: He⁺, 100 μA/cm² |
|                                  | (typical) Ar⁺, 10 μA/cm² |
The microanalysis facilities for use in materials science have been made available for collaborative research by members of universities or industry with ORNL staff members. The facilities include state-of-the-art electron microscopy, high voltage electron microscopy, field ion microscopy/atom probe, surface analysis, and nuclear microanalysis. The electron microscopy capabilities include analytical electron microscopy [energy dispersive X-ray spectroscopy (EDS), electron energy loss spectroscopy (EELS), and convergent beam electron diffraction (CBED)]. Surface analysis facilities include four Auger electron spectroscopy (AES) systems, and 0.4 and 5.0 Van de Graaff accelerators for Rutherford back-scattering and nuclear reaction techniques. An intermediate high voltage analytical electron microscope (300 kV) and an atom probe field ion microscope have been recently added to the SHaRE facilities.

**USER MODE**

User interactions are through collaborative research projects between users and researchers on the Materials Sciences Program at ORNL. Proposals are reviewed by an executive committee which consists of ORAU, ORNL, and university members. Current members are Drs. E. A. Kenik, Chairman, P. S. Sklad, R. J. Bayuzick, R. F. Davis, and R. E. Wiesehuegel. Proposals are evaluated on the basis of scientific excellence and relevance to DOE needs and current ORNL research. One ORNL staff member must be identified who is familiar with required techniques and will share responsibility for the project.

The SHaRE program provides technical help and limited travel expenses for academic participants through the Oak Ridge Associated Universities (ORAU).

**PERSONS TO CONTACT FOR INFORMATION**

<table>
<thead>
<tr>
<th>Name</th>
<th>Phone Number</th>
<th>FTS</th>
</tr>
</thead>
<tbody>
<tr>
<td>E. A. Kenik</td>
<td>(615) 574-5066</td>
<td>624-5066</td>
</tr>
<tr>
<td>Metals and Ceramics Division</td>
<td>Oak Ridge National Laboratory</td>
<td>Oak Ridge, Tennessee 37831</td>
</tr>
</tbody>
</table>

| A. Wohlpart     | (615) 576-3422      | 626-3422|
| Oak Ridge Associated Universities | P. O. Box 117 | Oak Ridge, Tennessee 37831 |
## Technical Data

<table>
<thead>
<tr>
<th>Facilities</th>
<th>Key Features</th>
<th>Operating Characteristics*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hitachi HU-1000 High Voltage Electron Microscope</td>
<td>Heating stages; in situ deformation stages; videorecording system; environmental cell</td>
<td>0.3-1.0 MeV; in situ studies electron irradiation studies; ten 4-h shifts per week</td>
</tr>
<tr>
<td>Philips EM400T/ FEG Analytical Electron Microscope (AEM)</td>
<td>EDS, EELS, CBEB, STEM; minimum probe diameter ( _1 ) nm</td>
<td>120 kV; ten 4-h shifts per week; structural and elemental microanalysis</td>
</tr>
<tr>
<td>JEM 120CX (AEM)</td>
<td>EDS, EELS, CBED, STEM; minimum probe diameter &lt;10 nm</td>
<td>120 kV; ten 4-h shifts per week; structural and elemental microanalysis</td>
</tr>
<tr>
<td>JEM 120C TEM</td>
<td>Polepiece for TEM of ferromagnetic materials</td>
<td>120 kV; ten 4-h shifts per week; structural microanalysis</td>
</tr>
<tr>
<td>PHI 590 Scanning Auger Electron Spectroscopy System</td>
<td>200 nm beam; fracture stage; RGA; depth profiling; elemental mapping</td>
<td>Surface analytical and segregation studies</td>
</tr>
<tr>
<td>Varian Scanning Auger Electron Spectroscopy System</td>
<td>5 micrometer beam; hot-cold fracture stage; RGA; depth profiling; elemental mapping</td>
<td>Surface analytical and segregation studies; gas-solid interaction studies</td>
</tr>
<tr>
<td>Dual Ion-Beam Accelerator Facilities</td>
<td>400 kV, 4 MV Van de Graaf accelerator; sputter profiling</td>
<td>Nuclear microanalysis; Rutherford backscattering; elemental analysis</td>
</tr>
<tr>
<td>Philips EM430T AEM</td>
<td>300 kV, STEM, EDS, EELS, CBED</td>
<td>Ten 4 h shifts/week; structural and elemental microanalysis</td>
</tr>
<tr>
<td>Atom Probe Field Ion Microscope</td>
<td>FOF atom probe, imaging atom probe, FIM, pulsed laser atom probe</td>
<td>Atomic resolution imaging; single atom analysis;</td>
</tr>
</tbody>
</table>

*Many instruments available off-hours (evenings, weekends) to qualified users.*
The Center operates a wide range of advanced surface chemistry, X-ray and electron-beam microanalytical equipment for the benefit of the University of Illinois materials research community and for the DOE Laboratories and Universities Programs. Equipment is selected to provide a spectrum of advanced microcharacterization techniques including microchemistry, microcrystallography, surface analysis, etc. A team of professionals runs the facility and its members facilitate the research.

USER MODE

Most of the research in the facility is funded by MRL contracts of U of Illinois faculty, and is carried out by graduate students, post-doctoral and faculty researchers and by the Center's own professional staff.

For the benefit of external users the system retains as much flexibility as possible. The preferred form of external usage is collaborative research through a contract with a faculty member associated with the MRL, or by direct negotiation with the management of the Center. Direct user access to the equipment is also possible, for trained individuals. In all cases, the research carried out by facility users has to be in the furtherance of DOE objectives.

The facility staff maintain training programs in the use of the equipment and teach associated techniques. An increasing part of the Center's activity is concerned with the development of new instruments and instrumentation.

A brochure describing the Center and its services is available.

PERSON TO CONTACT FOR INFORMATION

Dr. J. A. Eades, Coordinator
Center for Microanalysis of Materials
Materials Research Laboratory
University of Illinois
104 S. Goodwin
Urbana, Illinois 61801

(217)-333-8396
CENTER FOR MICROANALYSIS OF MATERIALS

<table>
<thead>
<tr>
<th>Instruments</th>
<th>Features and Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Imaging Secondary Ion Microprobe</td>
<td>Dual ion sources ($C_s^+$, $O_2^+$).</td>
</tr>
<tr>
<td>Cameca IMS 3f</td>
<td>1μm resolution.</td>
</tr>
<tr>
<td>Secondary Neutral Mass Spectrometer</td>
<td>Quantitative analysis,</td>
</tr>
<tr>
<td>Leybold Heraeus INA 3</td>
<td>Depth profiling.</td>
</tr>
<tr>
<td>Scanning Auger Microprobe</td>
<td>Resolution: SEM 30 nm, Auger 70 nm.</td>
</tr>
<tr>
<td>Physical Electronics 595</td>
<td>Windowless X-ray detector.</td>
</tr>
<tr>
<td>Scanning Auger Microprobe</td>
<td>Resolution: SEM 3 μm.</td>
</tr>
<tr>
<td>Physical Electronics 545</td>
<td></td>
</tr>
<tr>
<td>XPS</td>
<td></td>
</tr>
<tr>
<td>Physical Electronics 548</td>
<td>Double pass CMA. ESCA and Auger</td>
</tr>
<tr>
<td>Transmission Electron Microscope</td>
<td>Specimen temp. to 1550K</td>
</tr>
<tr>
<td>Philips EM430 (300kV)</td>
<td>EDS, EELS, STEM</td>
</tr>
<tr>
<td>Transmission Electron Microscope</td>
<td></td>
</tr>
<tr>
<td>Philips EM420 (120kV)</td>
<td>EDS (windowless), EELS, STEM,</td>
</tr>
<tr>
<td>Transmission Electron Microscope</td>
<td>Cathodoluminescence, Cold Stage (30K).</td>
</tr>
<tr>
<td>Philips EM400T (120kV)</td>
<td>EDS. Heating, cooling stages.</td>
</tr>
<tr>
<td>Transmission Electron Microscope</td>
<td>For environmental cell use.</td>
</tr>
<tr>
<td>JEOL 4000EX (400 kV)</td>
<td></td>
</tr>
<tr>
<td>Scanning Transmission E.M.</td>
<td>0.5 nm probe, field emission gun, EDS, EELS.</td>
</tr>
<tr>
<td>Vacuum Generators HBS (100kV)</td>
<td>5 nm resolution, EDX, channeling and backscattering patterns.</td>
</tr>
<tr>
<td>Scanning Electron Microscope</td>
<td>Two work stations, channeling</td>
</tr>
<tr>
<td>JEOL JSM 35C (35kV)</td>
<td></td>
</tr>
<tr>
<td>Rutherford Backscattering (in-house construction) (3 MeV)</td>
<td>Two work stations, channeling</td>
</tr>
<tr>
<td>X-ray Equipment</td>
<td>4-circle diffractometer.</td>
</tr>
<tr>
<td>Elliott 14 kW high brilliance source</td>
<td>Small angle camera. EXAFS.</td>
</tr>
<tr>
<td>Rigaku 12 kW source</td>
<td>Lang topography, Powder cameras, etc.</td>
</tr>
<tr>
<td>Several conventional sources</td>
<td></td>
</tr>
<tr>
<td>Rigaku D/Max-11B Computer Controlled Powder Diffractometer</td>
<td>4-circle diffractometer.</td>
</tr>
</tbody>
</table>

In addition to the main items listed above the Center also has other equipment: an electron microprobe, optical microscopes, a surface profiler, a microhardness tester, etc. Dark rooms and full specimen preparation facilities are available, including seven ion-milling stations, a micro-ion mill, electropolishing units, sputter coaters, a spark cutter, ultrasonic cutter, diamond saw, dimpler, etc.

The equipment is made available on a flexible week-by-week booking scheme; if professional help is required, operating hours are 8-5, except by special arrangement. Fully qualified users can and do use the equipment at any time of day. Several of the instruments are maintained in almost continuous (24 hour) use.
This program utilizes a new approach for fundamental materials research. The combined techniques of ion implantation doping, ion-induced mixing, and pulsed-laser processing are utilized to alter the near-surface properties of a wide range of solids in ultrahigh vacuum. Through in situ analysis by ion beam, surface, and bulk properties techniques, the fundamental materials interactions leading to these property changes are determined. Since both ion implantation doping and pulsed-laser annealing are nonequilibrium processing techniques, they can be used to produce new and often unique materials properties not possible with equilibrium fabrication techniques. This makes them ideal tools for fundamental materials research. They are equally useful for modifying surface properties for practical applications in areas such as friction, wear, corrosion, catalysis, surface hardness, solar cells, semiconducting devices, superconductors, etc.

This program has emphasis on long-range basic research. Consequently, most collaborative research involving scientists from industries, universities, and other laboratories has been the investigation of new materials properties possible with these processing techniques or the determination of the mechanisms responsible for observed property changes. In most instances such research projects identify definite practical applications and accelerate the transfer of these materials alteration techniques to processing applications.

COLLABORATIVE RESEARCH

User interactions are through mutually agreeable collaborative research projects between users and research scientists at ORNL which utilize the unique alteration/analysis capabilities of the SMAC facility. It should be emphasized that the goal of these interactions is to demonstrate the usefulness or feasibility of these techniques for a particular materials application and not to provide routine service alterations or analyses.

PERSON TO CONTACT FOR INFORMATION

S. P. Withrow  
Solid State Division  
Oak Ridge National Laboratory  
Oak Ridge, Tennessee  37831  
(615) 576-6719  
FTS  626-6719
Technical Data

<table>
<thead>
<tr>
<th>Accelerators</th>
<th>Operating Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5-MV positive ion Van de Graaff</td>
<td>0.1-3.2 MeV; H, D, $^4$He, $^3$He, and selected gases. Beam current ≤50 microamps</td>
</tr>
<tr>
<td>1.7-MV tandem</td>
<td>0.2-3.5 MeV H; 0.2-5.1 MeV $^3$He, $^4$He; negative ion sputtering source for heavy ion beams of most species to 7 MeV</td>
</tr>
<tr>
<td>10-200-KV high-current ion Implantation Accelerator</td>
<td>Essentially any species of ion; 1-3 mamps singly charged, ≤100 microamps doubly and triply charged</td>
</tr>
<tr>
<td>0.1-10-KeV Ion Gun</td>
<td>Gaseous species; ≤20 microamps</td>
</tr>
</tbody>
</table>

Lasers

- Pulsed Ruby Laser (0.6943 micrometer): 15-30 x 10^{-9} s pulse duration time; 10 joule/pulse output multimode; 2 joule/pulse output single mode (TEM_00)
- Pulsed Ruby Laser (0.6943 micrometer): 15-30 x 10^{-9} s pulse duration time; 8 joule/pulse output single mode (TEM_00)
- Pulsed Excimer Laser (0.249 micrometer): 20 x 10^{-9} s; 1.0 joule/pulse

Facilities

- UHV surface and near-surface analysis chambers: Several chambers; vacuums 10^{-6}-10^{-11} torr; multiple access ports; liquid helium cryostat; UHV goniometers (4-1300 K)
- In situ analysis capabilities: Ion scattering, ion channeling, ion-induced nuclear reactions and characteristic x rays; LEED, Auger, ion-induced Auger; electrical resistivity vs temperature
- Combined ion-beam and laser processing: Laser and ion beams integrated into same UHV chambers
- Dual simultaneous ion-beam irradiations: Combined accelerator irradiations
Optical techniques, primarily Raman spectroscopy and nonlinear optical spectroscopy, are being developed and used to study high-temperature interactions of materials exposed to combustion environments. Emphasis is on the in situ use of these techniques to identify chemical species present on surfaces during attack and the resultant effects on structural phases of the material under study. Both pulsed and continuous-wave lasers at various wavelengths throughout the visible and ultraviolet regions are available for excitation of Raman scattering, which can be analyzed with 1 and 2 dimensional photon counting detectors, multichannel diode array detectors, and gated detection. Combustion flow reactors and laboratory furnaces equipped with convenient optical accesses provide realistic environments for in situ measurements. Real-time measurements are complemented by post-exposure techniques such as Raman spectroscopy with sputtering and low-energy electron diffraction.

Nonlinear optical spectroscopies, in particular second harmonic generation, are being developed for the detection of monolayer and submonolayer coverages of surfaces. Picosecond Nd:YAG and dye lasers (10 pps) and a high repetition rate (1kHz) Nd:YAG laser provide pulsed excitation at a variety of wavelengths. Analysis of samples in UHV-based systems provides careful control over the high temperature modification of surfaces.

USER MODE

The materials program at the Combustion Research Facility has emphasized research into deposition and corrosion mechanisms using the techniques and apparatus described above. Interactions include: (1) collaborative research projects with outside users, and (2) technology transfer of new diagnostc approaches for the study of material attack. In initiating collaborative research projects, it is desirable to perform preliminary Raman analyses of typical samples and of reference materials to determine the suitability of Raman spectroscopy to the user's particular application. Users interested in exploring potential collaborations should contact the persons listed below. If further investigations appear reasonable, a brief written proposal is requested. Generally, visits of a week or more for external users provide an optimum period for information exchange and joint research efforts. Users from industrial, university, and government laboratories have been involved in these collaborative efforts. Results of these research efforts are published in the open literature.

PERSONS TO CONTACT FOR INFORMATION

FTS 532-2435

Gary B. Drummond, Ass't to the Director (8301) (415) 422-2697
FTS 532-2697

Sandia National Laboratories
Livermore, California 94550
## E-12
### TECHNICAL DATA

<table>
<thead>
<tr>
<th>Instruments</th>
<th>Key Features</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Raman Surface Analysis System</td>
<td>UHV Chamber; Raman system with Ar laser; triple spectrograph, diode array detector and 2-D imaging photon counting detector; Auger; sputtering capability.</td>
<td>Simultaneous Raman and sputtering. Raman system capable of detecting 2 nm thick oxides. Sample heating up to 1100°C.</td>
</tr>
<tr>
<td>Raman Microprobe</td>
<td>Hot stage; Raman system with Ar, Krypton lasers; scanning triple spectrometer.</td>
<td>1-2 micron spatial resolution. Hot stage can handle corrosive gases.</td>
</tr>
<tr>
<td>Raman High-Temperature Corrosion System</td>
<td>Furnace; Raman system with Ar, Krypton, Cu-vapor lasers Nd:YAG; triple spectrograph and diode array detector.</td>
<td>Pulsed lasers gated detection for blackbody background rejection. Furnace allows exposure to oxidizing, reducing, and sulfidizing environments.</td>
</tr>
<tr>
<td>Combustion Flow Reactors</td>
<td>Raman system with Ar, Krypton, Cu-vapor lasers; triple spectrograph and diode array detector.</td>
<td>Vapor and particulate injection into flames. Real-time measurements of deposit formation.</td>
</tr>
<tr>
<td>Electrochemical Surface Modification System</td>
<td>Electrochemical cell; Raman system with Ar, Krypton, Cu-vapor lasers; triple spectrograph and diode array detector.</td>
<td>Electrochemical cell with recirculating pump and nitrogen purge.</td>
</tr>
<tr>
<td>Nonlinear Optical Spectroscopy of Surfaces System</td>
<td>Picosecond Nd:YAG and dye lasers, 10 pps; UHV chamber equipped with LEED, Auger, sputtering, and quad. mass spectroscopy.</td>
<td>Monolayer and submonolayer detection of high temperature hydrogen and oxygen adsorption and nitrogen segregation on alloys.</td>
</tr>
<tr>
<td>Nonlinear Optical Spectroscopy of Electrochemical Systems</td>
<td>Nd:YAG laser, 1kHz rep rate; electrochemical cell.</td>
<td>Monolayer and submonolayer detection of lead, oxygen, and hydrogen adsorption at electrodes.</td>
</tr>
</tbody>
</table>
The Materials Preparation Center was established because of the unique capabilities for preparation, purification, fabrication and characterization of certain metals and materials that have been developed by investigators at the Ames Laboratory during the course of their basic research. Individuals within the Laboratory's Metallurgy and Ceramics Program are widely recognized for their work with very pure rare-earth, alkaline-earth and refractory metals. Besides strengthening materials research and development at the Ames Laboratory, the Center increases awareness by the research community of the scope and accessibility of this resource to universities, other government and private laboratories and provides appropriate transfer of unique technologies developed at the Center to private, commercial organizations.

Through these research efforts at Ames, scientists are now able to acquire very high-purity metals and alloys in single and polycrystalline forms, as well as the sophisticated technology necessary to satisfy many needs for special preparations of rare-earth, alkaline-earth, refractory and some actinide metals. The materials in the form and/or purity are not available from commercial suppliers, and through its activities the Center helps assure the research community access to materials of the highest possible quality for their research programs.

The Center consists of a Materials Preparation Section, an Analytical Section and the Materials Referral System and Hotline (MRSH). The Analytical Section has extensive expertise and capabilities for the characterization of materials, including complete facilities for chemical and spectrographic analyses, and selected services of this section are available to the research community. The purpose of MRSH is to accumulate information from all known National Laboratory sources regarding the preparation and characterization of materials and to make this information available to the scientific community.

**USER MODE**

Materials Preparation and Analytical Sections

Quantities of ultrapure rare-earth metals and alloys in single and polycrystalline forms are available. Special preparations of high-purity oxides and compounds are also available in limited quantities. Unique technologies developed at Ames Laboratory are used to prepare refractory metals in single and polycrystalline forms. In addition, certain alkaline-earth metals used as reducing agents are available. Complete characterization of these materials are provided by the Analytical Section. Materials availability and characterization information can be obtained from Frederick A. Schmidt, Director, Materials Preparation Center.
Materials Referral System and Hotline

The services of the Materials Referral System are available to the scientific community and inquiries should be directed to Tom Wessels, MRSN Manager, (515) 294-8900 or FTS 865-8900.

TECHNICAL DATA

Materials

<table>
<thead>
<tr>
<th>Scandium</th>
<th>Titanium</th>
<th>Magnesium</th>
<th>Thorium</th>
</tr>
</thead>
<tbody>
<tr>
<td>Yttrium</td>
<td>Vanadium</td>
<td>Calcium</td>
<td>Uranium</td>
</tr>
<tr>
<td>Lanthanum</td>
<td>Chromium</td>
<td>Strontium</td>
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</tr>
<tr>
<td>Cerium</td>
<td>Manganese</td>
<td>Barium</td>
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<td>Praseodymium</td>
<td>Zirconium</td>
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<tr>
<td>Neodymium</td>
<td>Niobium</td>
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<td></td>
</tr>
<tr>
<td>Samarium</td>
<td>Molybdenum</td>
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<td></td>
</tr>
<tr>
<td>Europium</td>
<td>Hafnium</td>
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<td></td>
</tr>
<tr>
<td>Gadolinium</td>
<td>Tantalum</td>
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<tr>
<td>Terbium</td>
<td>Tungsten</td>
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<tr>
<td>Dysprosium</td>
<td>Rhenium</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Holmium</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Erbium</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Thulium</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ytterbium</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lutetium</td>
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<td></td>
<td></td>
</tr>
</tbody>
</table>

PERSON TO CONTACT FOR INFORMATION

Frederick A. Schmidt, Director
Materials Preparation Center
121 Metals Development Building
Ames Laboratory
Ames, Iowa 50011

(515) 294-5236
The National Center for Electron Microscopy (NCEM) was formally established in the fall of 1981 as a component of the Materials and Molecular Research Division, Lawrence Berkeley Laboratory.

The NCEM provides unique facilities and advanced research programs in the United States for electron microscopy characterization of materials. Its mission is to carry out fundamental research and maintain state-of-the-art facilities and expertise. Present instrumentation at the Center includes a conventional 650-kV Hitachi electron microscope installed in 1969 in the Hearst Mining Building on the University of California Berkeley campus, a 1.6-MeV Kratos microscope dedicated largely for in-situ work, a 1-MeV JOEL atomic resolution microscope (ARM), a high-resolution feeder microscope (JEOL 200 CX), and a 200-kV analytical microscope (JEOL 200 CX) equipped with a thin window, high-angle X-ray detector, and an energy loss spectrometer. Facilities for image simulation, analysis and interpretation are also available to users.

USER MODE

Qualified microscopists with appropriate research projects of documented interest to DOE may use the Center without charge. Proprietary studies may be carried out on payment of full costs. Access to the Center may be obtained by submitting research proposals, which will be reviewed for Center justification by a Steering Committee (present external members are Drs. J. J. Hren, Chairman; J. M. Gibson, D. A. Howitt, F. Ponce, J. C. H. Spence, C. W. Allen, and L. E. Thomas; internal members are G. Thomas, T. L. Hayes, R. Gronsky, and K. H. Westmacott). A limited number of studies judged by the Steering Committee to be a sufficient merit can be carried out as a collaborative effort between a Center postdoctoral fellow, the outside proposer, and a member of the Center staff.

PERSON TO CONTACT FOR INFORMATION

Ms. Madeline Moore  
National Center for Electron Microscopy  
Mail Stop: 72-150  
Lawrence Berkeley Laboratory  
University of California  
Berkeley, California 94720  
(FTS) 451-5006, or  
(415) 486-5006
<table>
<thead>
<tr>
<th>Instruments</th>
<th>Key Features</th>
<th>Characterization</th>
</tr>
</thead>
<tbody>
<tr>
<td>KRATOS 1.5-MeV Electron Microscope</td>
<td>Resolution 3 Å (pt-pt) environmental cell; hot, cold, straining stages, CBED, video camera.</td>
<td>50-80 hrs/week 150-1500 kV range in 100 kV steps and continuously variable. LaB$_6$ filament. Max. beam current 70 amp/cm$^2$.</td>
</tr>
<tr>
<td>JEOL 1-MeV Atomic Resolution Microscope</td>
<td>Resolution &lt; 1.5 Å (pt-pt) over full voltage range. Ultrahigh resolution goniometer stage, $\pm 40^\circ$, biaxial tilt with height control.</td>
<td>50-80 hrs/week, 400 kV-1 MeV, LaB$_6$ filament, 3-mm diameter specimens.</td>
</tr>
<tr>
<td>Hitachi 650-kV Electron Microscope</td>
<td>General purpose resolution 20 Å environmental cell, straining stage.</td>
<td>Installed in 1969. Max. voltage 650 kV conventional HVEM, 3-mm diameter specimens.</td>
</tr>
<tr>
<td>JEOL 200 CX Electron Microscope</td>
<td>Dedicated high-resolution 2.4 Å (pt-pt) U.H. resolution goniometer stage only.</td>
<td>200 kV only, LaB$_6$ filament, 2.3-mm or 3-mm diameter specimens.</td>
</tr>
<tr>
<td>JEOL 200 CX dedicated Analytical Electron Microscope</td>
<td>Microdiffraction, CBED, UTW X-ray detector, high-angle X-ray detector, EELS spectrometer.</td>
<td>100 kV-200 kV LaB$_6$ filament, state-of-the-art resolution; 3-mm diameter specimens.</td>
</tr>
</tbody>
</table>
LOW-TEMPERATURE NEUTRON IRRADIATION FACILITY

Solid State Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

The Low-Temperature Neutron Irradiation Facility (LTNIF) is a user-oriented facility for the study of radiation effects in materials. It is available for qualified experiments at no cost to users. The LTNIF provides a combination of high radiation intensities and special environmental and testing conditions that have not been previously available in the U.S. A closed-cycle liquid-helium refrigerator and other cooling equipment allows samples to be held at temperatures between 3.2 and 800 K during irradiations and tests. In the initial configuration, the irradiation chamber fits into a vacant fuel element position in the reactor core to optimize fast neutron flux. Spectrum modifiers will be designed and constructed as needed to optimize gamma-ray or thermal-neutron flux. In many cases, experimental characterizations can be carried out in the irradiation cryostat. Alternatively, cold transfer to auxiliary equipment is available. The conditions available in the LTNIF are expected to prove useful in a wide variety of radiation effects studies, ranging from measurements of defect production and characterization in materials to the production of nonequilibrium phases of solids and the evaluation of structural materials for use in fusion reactors.

USER MODE

The LTNIF is operated as a user-oriented facility. In addition, a limited number of collaborative research projects will be undertaken by the staff. Time on the facility is assigned on the basis of proposals submitted in advance. Staff members are aided in the selection of user experiments by an advisory/program committee. Because of the special safety requirements of operating in a reactor, acceptance of proposals requires an evaluation by appropriate ORNL safety personnel in addition to the usual evaluation for scientific merit. Use of the reactor and cryostat is at no cost to users, but extensive use of shops and other support facilities must be paid by the user.

PERSONS TO CONTACT FOR INFORMATION

H. R. Kerchner (615) 574-6270
Solid State Division
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, Tennessee 37831

R. R. Coltman, Jr. (615) 574-6263
Solid State Division
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, Tennessee 37831
NATIONAL LOW-TEMPERATURE NEUTRON IRRADIATION FACILITY

Technical Data

Refrigeration: Minimum temperature, 3.2 K (low reactor power)
Capacity at 5 K, 70 W (removes nuclear heat generated in cryostat and a 100 g experiment at full reactor power)

Radiation (preliminary): Fast neutrons, \( (E > 0.1 \text{ MeV}) \times 10^{17} \text{ n/m}^2\text{s} \)
Thermal neutrons, \( 1.5 \times 10^{16} \text{ n/m}^2\text{s} \)
Gamma rays, 0.3 w/g (in Al)

Dimensions: Irradiation chamber, 38 mm diam x 250 mm long
Test chamber, 198 mm diam x 300 mm long
SECTION F

Summary of Funding Levels
SUMMARY OF FUNDING LEVELS

During the fiscal year ending September 30, 1986, the Materials Sciences total support level amounted to about $134.4 million in operating funds (budget outlays) and $12.0 million in equipment funds. The following analysis of costs is concerned only with operating funds (including SBIR) i.e., equipment funds which are expended primarily at Laboratories are not shown in the analysis. In contrast, equipment support for the Contract and Grant Research projects is included as part of the operating budget.

1. By Region of the Country

<table>
<thead>
<tr>
<th>Region</th>
<th>Contract and Grant Research (%) by $</th>
<th>Total Program (%) by $</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a) Northeast..............</td>
<td>37.8</td>
<td>28.1</td>
</tr>
<tr>
<td>(CT, DC, DE, MA, MD, ME,</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NJ, NH, NY, PA, RI, VT)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(b) South..................</td>
<td>11.2</td>
<td>18.9</td>
</tr>
<tr>
<td>(AL, AR, FL, GA, KY, LA,</td>
<td></td>
<td></td>
</tr>
<tr>
<td>MS, NC, SC, TN, VA, WV)</td>
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<td></td>
</tr>
<tr>
<td>(c) Midwest..............</td>
<td>21.8</td>
<td>28.9</td>
</tr>
<tr>
<td>(IA, IL, IN, MI, MN, MO,</td>
<td></td>
<td></td>
</tr>
<tr>
<td>OH, WI)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(d) West..................</td>
<td>29.2</td>
<td>24.1</td>
</tr>
<tr>
<td>(AZ, CO, KS, MT, NE, ND,</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NM, OK, SD, TX, UT, WY,</td>
<td></td>
<td></td>
</tr>
<tr>
<td>AK, CA, HW, ID, NV, OR, WA)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>100.0</td>
<td>100.0</td>
</tr>
</tbody>
</table>

2. By Discipline:

<table>
<thead>
<tr>
<th>Discipline</th>
<th>Contract and Grant Research (%) by $</th>
<th>Total Program (%) by $</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a) Metallurgy, Materials Science</td>
<td>57.6</td>
<td>36.4</td>
</tr>
<tr>
<td>Science, Ceramics</td>
<td>(Budget Activity Number 01-)</td>
<td></td>
</tr>
<tr>
<td>(b) Physics, Solid State</td>
<td>34.2</td>
<td>52.2</td>
</tr>
<tr>
<td>Science, Solid State Physics</td>
<td>(Budget Activity Numbers 02-)</td>
<td></td>
</tr>
</tbody>
</table>
SUMMARY OF FUNDING LEVELS

<table>
<thead>
<tr>
<th>Contract and Grant Research (% by $)</th>
<th>Total Program (% by $)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(c) Chemistry, Chemical Eng. (Budget Activity Numbers 03-)</td>
<td>8.2</td>
</tr>
<tr>
<td></td>
<td>100.0</td>
</tr>
</tbody>
</table>

3. By University, DOE Laboratory, and Industry:

(a) University Programs (including laboratories where graduate students are involved in research to a large extent, i.e., LBL, Ames and IL)........ 34.1

(b) DOE Laboratory Programs.............. 64.1

(c) Industry and Other.................. 1.8

100.0

4. By Laboratory and Contract and Grant Research:

<table>
<thead>
<tr>
<th>Total Program (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ames Laboratory</td>
</tr>
<tr>
<td>Argonne National Laboratory</td>
</tr>
<tr>
<td>Brookhaven National Laboratory</td>
</tr>
<tr>
<td>Idaho National Engineering Laboratory</td>
</tr>
<tr>
<td>Illinois, University of (Materials Research Laboratory)</td>
</tr>
<tr>
<td>Lawrence Berkeley Laboratory</td>
</tr>
<tr>
<td>Lawrence Livermore National Laboratory</td>
</tr>
<tr>
<td>Los Alamos National Laboratory</td>
</tr>
<tr>
<td>Oak Ridge National Laboratory</td>
</tr>
<tr>
<td>Pacific Northwest Laboratory</td>
</tr>
<tr>
<td>Sandia National Laboratory</td>
</tr>
<tr>
<td>Solar Energy Research Institute</td>
</tr>
<tr>
<td>Stanford Synchrotron Radiation Laboratory</td>
</tr>
</tbody>
</table>

Contract and Grant Research 18.6

100.0
SUMMARY OF FUNDING LEVELS

5. By Selected Areas of Research:

<table>
<thead>
<tr>
<th>Area</th>
<th>% of Prorated Projects&lt;sup&gt;a&lt;/sup&gt;</th>
<th>% of Program Funding&lt;sup&gt;a&lt;/sup&gt;</th>
<th>% of Individual Projects&lt;sup&gt;c&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(Total=425)</td>
<td>($134.4 million)</td>
<td>(Total=425)</td>
</tr>
<tr>
<td><strong>Materials</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ceramics (Crystalline)</td>
<td>15.3</td>
<td>12.6</td>
<td>21.6</td>
</tr>
<tr>
<td>Ferrous Alloys</td>
<td>8.3</td>
<td>4.9</td>
<td>16.7</td>
</tr>
<tr>
<td>Intermetallics</td>
<td>2.8</td>
<td>3.8</td>
<td>9.8</td>
</tr>
<tr>
<td>Polymers</td>
<td>3.9</td>
<td>2.6</td>
<td>6.8</td>
</tr>
<tr>
<td>Semiconductors</td>
<td>6.4</td>
<td>6.0</td>
<td>16.7</td>
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<tr>
<td><strong>Technique</strong></td>
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</tr>
<tr>
<td>Electron Microscopy</td>
<td>4.1</td>
<td>4.3</td>
<td>11.5</td>
</tr>
<tr>
<td>(Technique Development)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Neutron Scattering</td>
<td>5.9</td>
<td>19.1</td>
<td>16.2</td>
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<tr>
<td>Synchrotron Radiation</td>
<td>5.4</td>
<td>14.1</td>
<td>10.8</td>
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<tr>
<td>Theory</td>
<td>13.4</td>
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<td>33.4</td>
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<tr>
<td><strong>Phenomena</strong></td>
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<tr>
<td>Catalysis</td>
<td>2.2</td>
<td>2.2</td>
<td>6.6</td>
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<tr>
<td>Corrosion</td>
<td>3.6</td>
<td>2.3</td>
<td>9.9</td>
</tr>
<tr>
<td>Diffusion</td>
<td>4.2</td>
<td>3.4</td>
<td>16.9</td>
</tr>
<tr>
<td>Processing Science/Synthesis&lt;sup&gt;b&lt;/sup&gt;</td>
<td>8.3</td>
<td>7.4</td>
<td>34.6</td>
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<tr>
<td>Strength</td>
<td>8.0</td>
<td>4.4</td>
<td>27.8</td>
</tr>
<tr>
<td>Superconductivity</td>
<td>2.6</td>
<td>3.1</td>
<td>7.8</td>
</tr>
<tr>
<td><strong>Environment</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>High Temperature (&gt; 1200°K)</td>
<td>5.5</td>
<td>6.9</td>
<td>8.0</td>
</tr>
<tr>
<td>Radiation</td>
<td>6.4</td>
<td>9.4</td>
<td>10.6</td>
</tr>
<tr>
<td>Sulfur-Containing Gases</td>
<td>0.8</td>
<td>0.8</td>
<td>1.6</td>
</tr>
</tbody>
</table>

<sup>a</sup>The funding levels and projects percentage for various research categories were determined from the index listing in Section G and estimating the percentage from the project devoted to a particular subject. There is no overlap in the figures. For instance, funding for a project addressing creep of oxides would appear in the categories of ceramics, strength, and (possible) high temperature.

<sup>b</sup>Based on projects indexed in Section G under coatings, materials, preparation, powder metallurgy, solidification, surface treatments, thin films, and welding.

<sup>c</sup>Percentage of sum of individual projects involving the designated area of materials research.
SECTION G

Index of Investigators, Materials, Techniques, Phenomena, and Environment
<table>
<thead>
<tr>
<th>INVESTIGATORS</th>
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<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Aaron, W. S.</td>
<td>241</td>
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<tr>
<td>Abraham, M. M.</td>
<td>231</td>
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<tr>
<td>Abraham, L. A.</td>
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<tr>
<td>Adair, W. S.</td>
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<tr>
<td>Adams, B. L.</td>
<td>308</td>
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<tr>
<td>Adler, L.</td>
<td>443</td>
<td></td>
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<tr>
<td>Ahnlin, M.-K.</td>
<td>059</td>
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MATERIALS, TECHNIQUES, PHENOMENA, AND ENVIRONMENT

The numbers in parenthesis at the end of each listing of Abstract numbers gives for each topic the percentage of prorated projects, the percentage of funding, and the percentage of individual projects respectively. The prorated projects and the funding levels are based on estimates of the fractions of a given project devoted to the topic. The operating funds for fiscal year 1986 were $134,455,000, and the total number of projects was 425.

MATERIALS

Actinides-Metals, Alloys and Compounds

006, 008, 014, 048, 049, 054, 076, 164, 200, 205, 241, 244, 255, 323
349, 366, 417, 424, 508
(1.46, 1.43, 4.47)

Aluminum and its Alloys

019, 078, 106, 107, 109, 113, 126, 142, 175, 190, 201, 218, 232, 291
310, 316, 318, 321, 344, 356, 363, 427, 488, 497, 566
(2.00, 1.34, 5.88)

Alkali and Alkaline Earth Metals and Alloys

081, 164, 166, 206, 241, 373, 420
(0.38, 0.40, 1.65)

Amorphous State: Liquids

(0.96, 0.50, 2.35)

Amorphous State: Metallic Glasses

001, 043, 045, 075, 078, 106, 107, 123, 140, 191, 200, 201, 218, 223
232, 255, 277, 312, 321, 348, 365, 384, 406, 430, 449, 481, 510, 558
(2.16, 1.82, 6.59)

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

041, 047, 054, 081, 118, 119, 120, 152, 200, 227, 235, 277, 304, 317
333, 341, 348, 368, 406, 410, 415, 418, 426, 436, 469, 484, 496, 512
552
(2.12, 1.67, 6.82)

Amorphous State: Non-Metallic Glasses (Silicates)

012, 054, 116, 260, 262, 275, 303, 406, 418, 425, 436, 450, 477, 483
512
(1.29, 1.44, 3.53)
G-12

Carbides
012, 111, 115, 151, 168, 170, 178, 202, 229, 231, 234, 237, 303, 317
563
(2.05, 1.67, 6.82)

Cement and Concrete
448
(0.07, 0.02, 0.24)

Carbon and Graphite
146, 152, 163, 176, 232, 315, 353, 373, 458
(0.61, 0.24, 2.12)

Coal
110, 224
(0.28, 0.15, 0.47)

Composite Materials--Structural
013, 123, 151, 202, 220, 223, 232, 345, 351, 353, 425, 427, 482, 553
563, 567
(1.06, 0.76, 3.76)

Copper and its Alloys
001, 003, 009, 010, 013, 040, 061, 070, 071, 105, 109, 122, 126, 140
142, 170, 174, 201, 234, 236, 291, 305, 321, 332, 355, 360, 363, 387
395, 423, 441, 446, 459, 461, 472, 489, 501, 569
(3.20, 2.63, 8.94)

Dielectrics
(0.82, 0.34, 2.82)

Fast Ion Conductors (use Solid Electrolytes if more appropriate)
047, 054, 123, 338, 386, 436, 469, 473
(0.45, 0.45, 1.88)

Iron and its Alloys
001, 003, 004, 005, 014, 044, 060, 071, 075, 100, 105, 109, 113, 122
141, 142, 144, 146, 148, 174, 190, 201, 215, 216, 218, 221, 228, 255
261, 263, 290, 302, 305, 308, 309, 310, 311, 313, 316, 329, 334, 339
439, 440, 441, 442, 454, 459, 470, 472, 480, 487, 488, 489, 492, 502
509
(8.33, 4.93, 16.71)
Glasses (use terms under Amorphous State)
119, 192, 290, 348, 406, 433, 473
(0.52, 0.40, 1.65)

Hydrides
001, 007, 016, 021, 073, 076, 081, 112, 224, 241, 291
(0.71, 0.85, 2.59)

Intercalation Compounds
011, 024, 075, 130, 146, 152, 163, 223, 225, 373, 405, 428, 458, 474
(1.04, 0.85, 3.29)

Intermetallic Compounds
005, 008, 010, 011, 015, 017, 021, 023, 024, 040, 044, 049, 070, 072
075, 079, 108, 162, 164, 165, 174, 175, 201, 205, 216, 218, 219, 223
224, 225, 241, 318, 321, 348, 366, 380, 392, 394, 403, 430, 497, 568
(2.82, 3.83, 9.88)

Ionic Compounds
058, 120, 123, 125, 162, 192, 235, 341, 396, 457, 468, 480, 506
(0.94, 0.60, 3.06)

Layered Materials (including Superlattice Materials)
012, 013, 015, 016, 017, 045, 050, 051, 052, 054, 070, 076, 127, 165
240, 264, 277, 278, 327, 364, 393, 446, 458, 479
(1.65, 1.95, 5.65)

Liquids (use Amorphous State: Liquids)
131, 206, 326, 337, 395, 413
(0.78, 0.33, 1.41)

Metals and Alloys (other than those listed separately in this index)
014, 017, 019, 040, 042, 051, 055, 058, 061, 075, 079, 081, 124, 125
126, 127, 129, 141, 142, 145, 158, 162, 165, 166, 168, 170, 174, 176
178, 191, 201, 205, 215, 217, 218, 230, 234, 237, 239, 256, 277, 301
310, 326, 332, 348, 357, 366, 371, 374, 382, 421, 423, 430, 431, 447
452, 459, 473, 481, 494, 500, 552, 562, 567
(5.58, 5.41, 15.29)

Molecular Solids
057, 076, 117, 128, 131, 204, 243, 322, 336, 405, 411, 436, 444, 474
(1.39, 1.49, 3.29)

Nickel and its Alloys
005, 040, 043, 060, 071, 075, 079, 100, 105, 106, 107, 113, 122, 140
154, 201, 201, 218, 232, 237, 261, 291, 318, 321, 328, 340, 343, 344
357, 358, 366, 370, 374, 380, 394, 398, 401, 423, 441, 443, 463, 470
471, 472, 489
(3.72, 2.88, 10.59)
Nitrides
012, 021, 022, 056, 120, 178, 204, 229, 264, 303, 342, 346, 376, 388
397, 411, 412, 440, 482, 491, 498, 550, 554, 557
(1.67, 1.05, 5.65)

Oxides: Binary
021, 041, 047, 055, 058, 079, 081, 117, 118, 121, 144, 149, 151, 153
167, 201, 204, 218, 220, 229, 231, 235, 242, 244, 245, 260, 292, 301
453, 464, 466, 470, 471, 476, 480, 483, 486, 490, 494
(5.44, 4.29, 15.76)

Oxides: Non-Binary, Crystalline
021, 044, 049, 079, 116, 117, 127, 144, 147, 149, 151, 154, 218, 229
377, 386, 388, 396, 407, 410, 432, 435, 445, 448, 455, 485, 553, 557
562, 563, 564
(3.22, 2.12, 10.59)

Polymers
022, 084, 132, 177, 204, 224, 232, 236, 243, 255, 280, 307, 327, 345
351, 359, 362, 367, 409, 418, 422, 436, 438, 467, 469, 493, 496, 507
513
(3.91, 2.61, 6.82)

Platinum Metal Alloys (Platinum, Palladium, Rhodium, Iridium, Osmium, Ruthenium)
002, 015, 129, 142, 291, 335, 349, 355, 403, 478, 483, 485, 495, 511
(1.41, 0.70, 3.29)

Quantum Fluids and Solids
013, 047, 054, 128, 158, 161, 164, 166, 206, 223, 315, 322, 331, 352
369, 392, 403
(1.46, 1.19, 4.00)

Radioactive Waste Storage Materials (Hosts, Canister, Barriers)
116, 200, 263, 304, 386, 388, 410, 448, 457, 483
(0.71, 0.24, 2.35)

Rare Earth Metals and Compounds
001, 002, 003, 005, 006, 008, 010, 011, 014, 015, 018, 048, 054, 075
076, 141, 164, 166, 205, 223, 225, 235, 241, 323, 341, 372, 403, 408
416, 424, 468, 484, 504, 506
(2.35, 2.29, 8.00)
Refractory Metals (Groups VB and VI B)
003, 004, 006, 007, 010, 015, 016, 018, 021, 023, 040, 043, 073, 078
112, 140, 191, 228, 231, 234, 302, 358, 420
(1.69, 1.96, 5.41)

Semiconductor Materials - Elemental (including doped and amorphous phases)
012, 055, 078, 120, 122, 124, 127, 140, 155, 156, 157, 160, 162, 176
227, 230, 234, 237, 239, 240, 277, 278, 281, 324, 342, 347, 404, 414
415, 420, 446, 447, 480, 491, 565
(3.08, 3.28, 8.47)

Semiconductor Materials - Multicomponent (III-Vs. II-VIs. including doped and amorphous forms)
012, 017, 018, 108, 119, 122, 124, 127, 130, 131, 155, 156, 162, 172
227, 276, 278, 281, 347, 355, 356, 368, 401, 407, 411, 412, 414, 415
418, 431, 435, 447, 462, 470, 490, 511
(3.34, 2.69, 8.47)

Solid Electrolytes
076, 079, 084, 120, 231, 338, 386, 469, 473
(0.49, 0.45, 2.12)

Structural Ceramics (Si-N. SiC. SIALON. Zr-O (transformation toughened))
022, 024, 111, 113, 115, 118, 121, 147, 151, 201, 202, 217, 220, 222
242, 245, 255, 256, 303, 330, 342, 346, 376, 384, 389, 397, 412, 445
451, 464, 480, 482, 486, 491, 498, 550, 553, 556, 562, 563, 564
(3.13, 2.55, 9.65)

Superconductors (also see Superconductivity in the Phenomena index and Theory in the Techniques index)
003, 013, 015, 020, 047, 048, 056, 057, 072, 075, 079, 125, 158, 161
162, 164, 166, 174, 215, 223, 224, 226, 280, 302, 323, 349, 355, 364
391, 392, 406, 493, 504
(2.56, 3.10, 7.76)

Surfaces and Interfaces
002, 013, 014, 019, 024, 041, 044, 045, 050, 052, 054, 059, 061, 070
076, 077, 081, 127, 149, 151, 153, 162, 163, 165, 168, 173, 176, 202
290, 291, 292, 312, 318, 343, 365, 375, 380, 395, 418, 428, 446, 447
451, 456, 479
(4.75, 6.16, 13.88)

Synthetic Metals
057, 307, 364, 367, 393, 429, 493
(0.80, 0.71, 1.65)
Transition Metals and Alloys (other than those listed separately in this index)
013, 018, 021, 023, 043, 074, 079, 168, 176, 215, 218, 305, 323, 366
(0.80, 1.21, 3.29)
TECHNIQUES

Acoustic Emission
071, 148, 261, 354, 481, 560
(0.56, 0.64, 1.41)

Auger Electron Spectroscopy
001, 004, 012, 016, 024, 050, 052, 060, 061, 072, 073, 078, 106, 107
324, 357, 381, 387, 398, 412, 421, 431, 479, 495, 497, 510
(2.24, 2.57, 9.41)

Bulk Analysis Methods (other than those listed separately in this
index, e.g., ENDOR, muon spin rotation, etc.)
006, 007, 010, 061, 200, 205, 226, 497
(0.54, 0.42, 1.88)

Computer Simulation
005, 018, 041, 050, 052, 054, 055, 058, 071, 156, 157, 161, 162, 163
174, 175, 201, 204, 216, 218, 228, 233, 243, 245, 255, 262, 275, 291
303, 313, 326, 327, 331, 342, 349, 365, 368, 381, 382, 389, 396, 400
406, 419, 436, 450, 459, 473, 476, 481, 483, 488, 490, 501, 511
(4.45, 3.30, 12.94)

Chemical Vapor Deposition (all types)
201, 218, 276, 278, 281, 347, 364, 435
(0.54, 0.49, 1.88)

Dielectric Relaxation
230, 338, 366, 377
(0.19, 0.07, 0.94)

Deep Level Transient Spectroscopy
347, 407, 435
(0.19, 0.06, 0.71)

Electron Diffraction (Technique development, not usage, for all
types--LEED, RHEED, etc.)
279, 301, 320, 381, 479, 481, 495, 514
(1.20, 1.42, 5.18)

Electron Energy Loss Spectroscopy (EELS)
001, 012, 024, 043, 044, 048, 106, 107, 111, 115, 140, 141, 143, 217
237, 256, 279, 301, 319, 320, 332, 371, 374, 375, 397, 416, 431, 475
490, 497, 514
(2.12, 2.08, 7.29)
Elastic Constants
049, 050, 072, 112, 126, 175, 201, 336, 353, 354, 377, 443, 452, 478
(0.73, 0.51, 3.29)

Electrochemical Methods
005, 024, 057, 058, 059, 060, 105, 131, 132, 160, 165, 168, 170, 242
487, 511, 558, 566
(2.92, 2.25, 7.53)

Electron Microscopy (technique development for all types)
002, 003, 004, 041, 043, 044, 056, 070, 106, 107, 109, 110, 111, 113
115, 119, 122, 140, 141, 142, 143, 146, 148, 172, 174, 175, 190, 200
201, 202, 202, 217, 218, 219, 220, 227, 228, 234, 240, 256, 260, 301
358, 363, 375, 432, 439, 441, 480
(4.14, 4.23, 11.53)

Electron Spectroscopy for Chemical Analysis (ESCA)
023, 024, 050, 052, 108, 151, 202, 497
(0.21, 0.24, 1.88)

Electron Spin Resonance or Electron Paramagnetic Resonance
059, 117, 120, 172, 235, 280, 338, 407, 484
(0.64, 0.49, 2.12)

Extended X-Ray Absorption Fine Structure (EXAFS and XANES)
023, 049, 070, 071, 072, 073, 084, 116, 125, 160, 178, 200, 255, 304
312, 313, 338, 366, 375, 410, 418, 421, 428, 432, 436, 483, 484, 493
494, 497, 506
(1.67, 1.40, 7.29)

Field Emission and Field Ion Microscopy
024, 190, 217, 256, 279, 358, 456, 463
(0.75, 0.49, 1.88)

High Pressure (Technique development of all types)
015, 047, 060, 201, 205, 245, 484
(0.31, 0.63, 1.65)

Ion or Molecular Beams
043, 108, 218, 222, 238, 240, 305, 324, 355, 358, 551
(0.96, 0.89, 2.59)

Ion Channeling, or Ion Scattering (including Rutherford and other
ion scattering methods)
042, 043, 044, 045, 218, 222, 235, 238, 239, 240, 277, 302, 324, 374
391, 510
(0.94, 1.98, 3.76)
Internal Friction (also see Ultrasonic Testing and Wave Propagation)
004, 006, 007, 016, 110, 112, 126, 338, 377, 452, 469
(0.61, 0.25, 2.59)

Infrared Spectroscopy (also see Raman Spectroscopy)
024, 059, 060, 117, 151, 155, 176, 204, 227, 229, 230, 275, 277, 332
338, 359, 362, 367, 373, 377, 386, 407, 426, 436, 450, 469, 482
(1.58, 1.41, 6.35)

Laser Spectroscopy (scattering and diagnostics)
061, 100, 132, 155, 176, 177, 192, 227, 245, 278, 278, 281, 290, 292
306, 325, 337, 341, 404, 409, 413, 422, 426, 447, 465, 468, 481, 491
512
(2.94, 1.65, 6.82)

Magnetic Susceptibility
008, 009, 013, 015, 048, 049, 050, 052, 057, 125, 171, 205, 226, 280
323, 392, 393, 414, 478, 493
(1.60, 1.73, 4.71)

Molecular Beam Epitaxy
050, 052, 108, 124, 127, 276, 278, 419
(0.38, 0.29, 1.88)

Mossbauer Spectroscopy
048, 059, 148, 174, 235, 312, 313, 373, 405, 444, 474, 484, 506
(0.73, 0.53, 3.06)

Neutron Scattering: Elastic (Diffraction)
011, 016, 017, 047, 052, 057, 058, 074, 075, 076, 079, 112, 128, 130
205, 223, 224, 225, 243, 352, 353, 390, 391, 432, 458
(1.69, 2.96, 5.88)

Neutron Scattering: Inelastic
007, 011, 016, 047, 058, 059, 073, 074, 075, 076, 128, 130, 152, 223
224, 225, 243, 352, 373, 377, 444, 449, 452, 508
(1.67, 2.64, 5.65)

Neutron Scattering: Small Angle
040, 047, 130, 170, 224, 226, 243, 291, 312, 363, 378, 433, 434, 467
486
(1.27, 1.21, 3.53)

Nuclear Magnetic Resonance and Ferromagnetic Resonance
016, 059, 117, 129, 156, 157, 158, 177, 178, 280, 312, 315, 338, 362
367, 393, 403, 433, 436, 469, 482, 504
(1.86, 1.03, 5.18)
Optical Absorption
  014, 024, 059, 192, 264, 409
  (0.35, 0.30, 1.41)

Perturbed Angular Correlation and Nuclear Orientation
  445
  (0.24, 0.04, 0.24)

Photoluminescence
  131, 132, 192, 276, 341, 347, 435, 450, 468
  (0.64, 0.32, 2.12)

Positron Annihilation (including slow positrons)
  040, 078, 291, 430
  (0.31, 0.44, 0.94)

Powder Consolidation (including sintering, hot pressing, dynamic compaction, laser assisted, etc., of metals and ceramics, use this item in the Phenomena index)
  079, 118, 121, 147, 151, 153, 202, 220, 241, 372, 408, 553, 557
  562, 563, 567
  (1.76, 1.18, 4.00)

Powder Synthesis (including preparation, characterization, or pre-consolidation behavior, use this item in the Phenomena index)
  023, 045, 072, 079, 118, 121, 147, 151, 153, 202, 220, 242, 392, 509
  (0.96, 0.95, 3.29)

Raman Spectroscopy (also see Infrared Spectroscopy)
  024, 059, 060, 125, 192, 204, 230, 242, 260, 263, 264, 276, 290, 292
  319, 335, 367, 373, 386, 401, 436, 447, 449, 484
  (1.51, 1.40, 5.65)

Rapid Solidification Processing (also see Solidification: Rapid in the Phenomena index)
  002, 048, 106, 107, 190, 191, 227, 239, 277, 313, 321, 360, 365, 455
  (0.94, 1.00, 3.29)

Surface Analysis Methods (other than those listed separately in this index, e.g., ESCA, Slow Positrons, X-Ray, etc.)
  001, 004, 014, 024, 051, 052, 061, 070, 078, 108, 112, 127, 132, 168
  073, 176, 192, 216, 238, 239, 255, 262, 275, 305, 312, 319, 332, 335
  371, 421, 424, 431, 446, 479, 503, 567
  (2.52, 2.27, 8.47)

Spinodal Decomposition
  174, 175, 217, 256, 360, 498
  (0.26, 0.23, 1.41)


Specific Heat
008, 015, 016, 048, 049, 125, 164, 205, 280, 312, 315, 369, 484
(0.99, 0.81, 3.06)

Sputtering
001, 012, 050, 051, 061, 076, 079, 108, 158, 241, 302, 372, 391, 408
416, 449, 510
(0.94, 1.09, 4.00)

Synchrotron Radiation
007, 014, 017, 024, 040, 048, 051, 053, 070, 077, 079, 081, 084, 124
159, 172, 204, 216, 234, 243, 255, 275, 304, 333, 360, 382, 410, 412
418, 420, 421, 422, 424, 431, 432, 436, 446, 470, 483, 493, 494, 506
(2.96, 4.05, 9.88)

Surface Treatment and Modification (including ion implantation, laser processing, electron beam processing, sputtering, etc., see Chemical Vapor Deposition)
045, 052, 078, 081, 105, 106, 107, 109, 153, 154, 190, 191, 192, 202
218, 222, 226, 227, 229, 235, 238, 239, 240, 242, 276, 277, 312, 317
324, 371, 383, 388, 412, 451, 455, 490, 558, 562
(2.49, 2.96, 8.94)

Synthesis
021, 022, 023, 057, 059, 079, 084, 127, 178, 242, 245, 307, 318, 323
372, 386, 408, 457, 493
(1.74, 1.67, 4.47)

Theory: Defects and Radiation Effects
040, 041, 042, 055, 072, 126, 200, 218, 228, 233, 263, 304, 317, 338
363, 396, 404, 410, 411, 426, 435
(1.25, 1.41, 4.94)

Theory: Electronic and Magnetic Structure
008, 016, 018, 023, 040, 049, 054, 055, 059, 080, 146, 162, 192, 205
215, 233, 276, 280, 327, 349, 366, 396, 406, 411, 415, 417, 430, 432
437, 444, 462, 497, 504, 505, 508
(2.42, 1.70, 8.24)

Theory: Non-Destructive Evaluation
009, 312
(0.09, 0.15, 0.47)

Theory: Surface
019, 019, 055, 061, 080, 149, 160, 162, 163, 215, 220, 233, 320, 365
381, 419, 423, 462, 483, 490, 514
(1.53, 1.33, 4.94)
| Theory: Superconductivity | 020, 048, 054, 080, 158, 161, 162, 205, 215, 349, 429, 493, 504 (0.99, 0.92, 3.06) |
| Theory: Thermodynamics, Statistical Mechanics, and Critical Phenomena | 005, 058, 059, 080, 128, 145, 156, 174, 175, 177, 201, 206, 220, 227, 228, 233, 243, 244, 245, 308, 327, 331, 336, 349, 352, 365, 370, 381, 398, 437, 452, 473, 478, 480, 496, 507 (2.78, 2.05, 8.47) |
| Thermal Conductivity | 123, 206, 322, 455 (0.52, 0.23, 0.94) |
| Ultrasonic Testing and Wave Propagation | 005, 009, 100, 105, 112, 126, 310, 322, 338, 443, 452, 491, 492 (1.18, 0.58, 3.06) |
| Vacuum Ultraviolet Spectroscopy | 014, 051, 160, 373, 383, 421, 494, 556 (0.64, 0.55, 1.88) |
| Work Functions | 431 (0.02, 0.00, 0.24) |
X-Ray Scattering (small angle)
(0.94, 0.61, 3.06)

X-Ray Scattering (other than crystallography)
017, 047, 051, 077, 160, 216, 243, 255, 360, 363, 374, 405, 416, 470
472, 474, 513, 513, 555, 559
(1.74, 1.91, 4.71)

X-Ray Photoelectron Spectroscopy
007, 016, 021, 023, 024, 049, 051, 060, 070, 081, 084, 160, 237, 262
332, 357, 359, 366, 395, 412, 418, 424, 431, 432, 450, 490, 497, 497
(1.44, 1.48, 6.59)
PHENOMENA

Catalysis
024, 047, 059, 081, 129, 146, 162, 178, 232, 237, 239, 242, 245, 255
301, 332, 365, 371, 374, 375, 423, 456, 470, 483, 485, 495, 500, 552
(2.16, 2.15, 6.59)

Channeling
003, 218, 239, 277, 302
(0.21, 0.42, 1.18)

Coatings (also see Surface Phenomena in this index)
024, 045, 160, 161, 165, 241, 264, 359, 412
(0.82, 1.01, 2.12)

Colloidal Suspensions
117, 121, 151, 177, 202, 220, 306, 337, 346, 359, 389, 466, 482
(0.68, 0.50, 3.06)

Conduction: Electronic
041, 057, 058, 084, 119, 129, 131, 215, 229, 236, 276, 280, 302, 307
327, 347, 349, 367, 368, 383, 404, 407, 414, 415, 417, 429, 432, 435
462, 468, 469, 490, 493, 510
(2.45, 1.85, 8.00)

Conduction: Ionic
(0.82, 0.59, 2.82)

Constitutive Equations
201
(0.02, 0.07, 0.24)

Corrosion: Aqueous (e.g., crevice corrosion, pitting, etc., also see Stress Corrosion)
009, 060, 071, 105, 168, 175, 261, 262, 277, 329, 335, 379, 395, 398
401, 440, 558, 566
(1.53, 1.24, 4.24)

Corrosion: Gaseous (e.g., oxidation, sulfidation, etc.)
023, 044, 058, 071, 144, 154, 167, 216, 255, 290, 319, 357, 370, 371
387, 401, 440, 441, 464, 552
(1.72, 1.03, 4.71)

Corrosion: Molten Salt
058, 260, 340, 464
(0.42, 0.14, 0.94)
Critical Phenomena (including order-disorder, also see Thermodynamics and Phase Transformations in this index)
016, 054, 058, 075, 077, 079, 156, 164, 231, 243, 245, 255, 306, 313
315, 322, 326, 331, 336, 337, 352, 360, 377, 381, 403, 413, 414, 422
452, 458, 465, 466, 496
(2.33, 1.52, 7.76)

Crystal Structure and Periodic Atomic Arrangements
021, 055, 057, 075, 077, 079, 142, 143, 145, 146, 162, 174, 175, 204
375, 376, 386, 388, 397, 407, 410, 419, 420, 428, 431, 432, 435, 436
448, 450, 452, 455, 458, 469, 470, 476, 482, 483, 486, 490, 497, 498
500, 506, 508, 510
(4.07, 3.47, 14.12)

Diffusion: Bulk
006, 007, 016, 040, 041, 044, 079, 105, 112, 130, 167, 218, 229, 243
472, 473, 477, 478, 483, 510, 511
(2.09, 1.58, 8.24)

Diffusion: Interface
017, 041, 044, 070, 072, 153, 165, 168, 170, 218, 230, 260, 262, 292
312, 324, 326, 348, 358, 380, 382, 383, 387, 415, 433, 445, 453, 465
471
(1.79, 1.47, 6.82)

Diffusion: Surface
149, 279, 337, 365, 371, 453, 456, 495
(0.42, 0.31, 1.88)

Dislocations
004, 017, 113, 115, 123, 142, 172, 174, 175, 201, 217, 218, 228, 256
291, 310, 329, 344, 347, 382, 420, 480, 481, 495, 502
(1.18, 1.23, 5.88)

Dynamic Phenomena
054, 055, 076, 156, 206, 223, 224, 225, 233, 243, 290, 292, 310, 320
331, 337, 341, 355, 365, 377, 400, 405, 406, 411, 422, 452, 465, 466
470, 474, 512, 514
(2.71, 2.44, 7.53)

Electronic Structure - Metals including amorphous forms
007, 014, 016, 018, 021, 023, 040, 048, 054, 078, 081, 124, 125, 129
201, 205, 215, 229, 233, 312, 335, 349, 366, 372, 408, 417, 421, 424
430, 437, 446, 497, 500, 504, 505
(2.59, 2.05, 8.24)
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<td><strong>Electronic Structure - Non-metals including amorphous forms</strong></td>
<td>049, 078, 108, 120, 124, 131, 162, 327, 336, 341, 396, 404, 411, 414, 415, 432, 435, 446, 462, 493, 505, 512</td>
<td>(1.41, 0.84, 5.18)</td>
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<td><strong>Erosion</strong></td>
<td>109, 427, 439</td>
<td>(0.19, 0.05, 0.71)</td>
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<td><strong>Hydrogen Attack</strong></td>
<td>111, 113, 277, 305, 442, 456</td>
<td>(0.42, 0.31, 1.41)</td>
</tr>
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<td><strong>Ion Beam Mixing</strong></td>
<td>042, 043, 045, 222, 238, 239, 242, 317</td>
<td>(0.61, 1.76, 1.88)</td>
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<td><strong>Laser Radiation Heating (annealing, solidification, surface treatment)</strong></td>
<td>061, 105, 108, 109, 141, 190, 191, 192, 227, 234, 238, 239, 277, 365, 383, 455, 481</td>
<td>(1.06, 1.80, 4.00)</td>
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<td><strong>Magnetism</strong></td>
<td>003, 008, 011, 013, 015, 018, 048, 052, 054, 075, 077, 081, 120, 125, 146, 152, 156, 156, 166, 215, 223, 225, 233, 323, 327, 349, 372, 392, 393, 403, 408, 414, 417, 444, 479, 494, 567</td>
<td>(2.96, 2.93, 8.71)</td>
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<tr>
<td><strong>Martensitic Transformations and Transformation Toughening</strong></td>
<td>011, 017, 148, 174, 377, 428</td>
<td>(0.33, 0.27, 1.41)</td>
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<td><strong>Mechanical Properties and Behavior: Constitutive Equations</strong></td>
<td>100, 113, 201, 303, 316, 344, 346, 353, 378, 384, 427, 477, 488, 489</td>
<td>(0.89, 0.44, 3.29)</td>
</tr>
<tr>
<td><strong>Mechanical Properties and Behavior: Creep</strong></td>
<td>044, 115, 218, 263, 308, 309, 316, 334, 339, 344, 363, 378, 397, 434, 461, 471, 481, 486, 488, 489, 498, 562</td>
<td>(1.44, 0.63, 5.18)</td>
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### Mechanical Properties and Behavior: Fatigue
009, 113, 148, 174, 175, 218, 228, 309, 311, 339, 379, 394, 402, 425
434, 439, 461, 477, 488, 492, 502
(1.36, 0.71, 4.94)

### Mechanical Properties and Behavior: Flow Stress
004, 115, 174, 175, 201, 310, 344, 345, 351, 384, 402, 420, 425, 427
467, 488, 498
(1.18, 0.59, 4.00)

### Mechanical Properties and Behavior: Fracture and Fracture Toughness
004, 009, 100, 113, 115, 141, 147, 148, 154, 173, 174, 175, 202, 218
220, 228, 275, 303, 309, 311, 329, 339, 345, 351, 353, 354, 378, 395
397, 402, 425, 439, 440, 441, 451, 480, 481, 486, 488, 491, 498, 550
553, 563
(3.18, 2.03, 10.35)

### Materials Preparation and Characterization: Ceramics
021, 041, 044, 049, 079, 111, 118, 119, 121, 127, 141, 147, 149, 151
333, 342, 346, 359, 376, 386, 389, 397, 407, 412, 426, 435, 448, 450
451, 455, 457, 466, 469, 476, 477, 482, 483, 486, 498, 512
(2.99, 2.32, 12.71)

### Materials Preparation and Characterization: Glasses
041, 235, 275, 312, 346, 436, 477
(0.35, 0.52, 1.65)

### Materials Preparation and Characterization: Metals
003, 010, 013, 017, 021, 043, 056, 061, 079, 100, 125, 127, 141, 142
145, 168, 170, 171, 174, 175, 190, 191, 201, 217, 219, 231, 232, 241
256, 302, 312, 318, 323, 363, 364, 372, 380, 408, 500, 510
(2.28, 2.48, 9.65)

### Materials Preparation and Characterization: Polymers
084, 177, 243, 422, 436, 493
(0.38, 0.39, 1.41)

### Materials Preparation and Characterization: Semiconductors
012, 017, 124, 127, 156, 171, 172, 231, 276, 278, 312, 324, 347, 368
404, 431, 435, 490, 511, 565
(1.67, 1.14, 4.71)

### Nondestructive Testing and Evaluation
005, 009, 152, 312, 354, 420, 434, 443, 492, 562
(0.78, 0.41, 2.35)
Phonons
011, 013, 018, 076, 120, 123, 130, 155, 164, 223, 224, 225, 233, 312
320, 336, 355, 371, 373, 377, 411, 426, 450, 452, 462, 475, 514
(1.72, 1.83, 6.35)

Photothermal Effects
281, 404
(0.12, 0.12, 0.47)

Photovoltaic Effects
012, 131, 227, 281, 347, 468, 490
(0.59, 0.65, 1.65)

Phase Transformations (also see Thermodynamics and Critical Phenomena in this index)
003, 005, 008, 018, 040, 049, 057, 074, 075, 077, 079, 111, 129, 130
131, 142, 145, 146, 153, 162, 174, 175, 190, 201, 204, 216, 217, 218
221, 224, 225, 256, 280, 315, 322, 334, 336, 355, 360, 373, 377, 384
403, 413, 421, 428, 431, 438, 445, 446, 452, 465, 470, 480, 498, 506
509
(3.53, 3.58, 13.41)

Precipitation
002, 003, 006, 016, 119, 121, 122, 141, 142, 146, 174, 175, 190, 217
218, 228, 232, 256, 263, 306, 328, 330, 376, 388, 389, 398, 434, 442
450, 498, 502
(1.67, 0.93, 7.29)

Point Defects
016, 040, 041, 042, 044, 055, 078, 122, 126, 128, 149, 158, 172, 192
216, 218, 219, 234, 236, 263, 310, 338, 347, 358, 375, 382, 396, 411
426, 432, 435, 445, 453, 478, 481, 487
(2.38, 2.72, 8.47)

Powder Consolidation (including sintering, hot pressing, dynamic compaction, laser assisted, etc., of metals and ceramics)
079, 106, 107, 118, 151, 153, 202, 202, 220, 318, 333, 346, 383, 386
389, 426, 455, 476, 482, 486, 498
(1.01, 0.64, 4.94)

Powder Synthesis (including preparation, characterization, or pre-consolidation behavior, see same item under Technique index)
021, 022, 079, 106, 107, 118, 151, 153, 202, 220, 231, 242, 318, 346
359, 386, 389, 392, 433, 455, 466, 482, 498, 509, 568
(1.62, 1.62, 5.88)
Radiation Effects (use specific effects, e.g., Point Defects and Environment index)
042, 045, 056, 061, 122, 158, 200, 217, 218, 234, 236, 256, 263, 301
404, 435, 481
(1.01, 1.51, 4.00)

Recrystallization and Recovery
116, 119, 128, 239, 263, 344, 364, 394, 449, 461, 510
(0.99, 0.44, 2.59)

Residual Stress
009, 353, 451, 491, 492
(0.38, 0.17, 1.18)

Rheology
121, 177, 362
(0.35, 0.22, 0.71)

Stress-Corrosion
001, 009, 060, 071, 105, 148, 175, 261, 395, 398, 401, 440, 477
(0.80, 0.82, 3.06)

Solidification (conventional)
002, 010, 100, 315, 334, 337, 413, 454, 557
(0.78, 0.28, 2.12)

SOL-GEL Systems
117, 151, 220, 232, 275, 306, 553
(0.49, 0.49, 1.65)

Solidification (rapid)
002, 047, 106, 107, 109, 190, 191, 226, 233, 239, 312, 321, 326, 387
455, 481, 510
(1.15, 1.26, 4.00)

Surface Phenomena: Chemisorption (binding energy greater than 1eV)
001, 014, 073, 078, 081, 112, 124, 129, 149, 167, 168, 170, 178, 215
237, 301, 305, 319, 320, 332, 359, 365, 369, 401, 418, 419, 421, 423
446, 447, 456, 475, 479, 503, 514
(2.52, 2.23, 8.24)

Surface Phenomena: Physiosorption (binding energy less than 1eV)
019, 050, 061, 077, 081, 279, 281, 315, 319, 332, 359, 419, 431, 447
475
(0.99, 1.03, 3.53)
Surface Phenomena: Structure
301, 320, 332, 355, 357, 359, 360, 375, 395, 418, 419, 421, 430, 431
438, 451, 462, 470, 495, 503, 514
(2.35, 2.09, 8.24)

Surface Phenomena: Thin Films (also see Coatings in this index)
047, 050, 051, 052, 056, 070, 081, 108, 124, 132, 155, 160, 161, 162
168, 173, 222, 240, 242, 264, 279, 290, 292, 301, 302, 312, 315, 320
337, 348, 357, 359, 412, 416, 438, 449, 450, 453, 479, 483, 487, 490
495, 510, 514
(3.55, 3.75, 10.59)

Short-range Atomic Ordering
176, 215, 216, 243, 262, 313, 428, 494, 503
(0.68, 0.75, 2.12)

Superconductivity
003, 013, 015, 020, 048, 050, 056, 057, 072, 155, 158, 161, 162, 164
174, 205, 226, 236, 302, 312, 349, 391, 392, 417, 493, 504, 569
(2.14, 2.27, 6.35)

Thermodynamics (also see Critical Phenomena and Phase
Transformations in this index)
005, 023, 058, 073, 125, 140, 145, 164, 166, 170, 174, 190, 201, 206
244, 315, 326, 328, 330, 331, 334, 336, 356, 369, 397, 445, 450, 458
472, 478, 480, 482, 496, 504, 507, 509, 511, 550
(3.29, 1.79, 8.94)

Transformation Toughening (metals and ceramics - see Martensitic
Transformation and Transformation Toughening in this Index)
141, 330, 377, 445, 480, 482
(0.24, 0.13, 1.41)

Valence Fluctuations
014, 048, 164, 205, 323, 349, 424, 484
(0.73, 0.60, 1.88)

Wear
109, 141, 222
(0.14, 0.23, 0.71)

Welding
100, 175, 221, 334, 442, 454
(0.42, 0.28, 1.41)
ENVIRONMENT

Aqueous
060, 105, 117, 121, 168, 175, 261, 262, 275, 301, 329, 337, 351, 379
395, 457, 487
(3.60, 2.63, 4.00)

Gas: Hydrogen
004, 007, 016, 073, 111, 112, 113, 144, 167, 228, 290, 291, 292, 309
354, 369, 374, 402, 441, 442, 464, 478
(4.16, 2.70, 5.18)

Gas: Oxidizing
041, 044, 148, 219, 260, 290, 292, 301, 318, 319, 339, 357, 370, 371
387, 401, 412, 441, 464
(2.66, 2.35, 4.47)

Gas: Sulphur-Containing
044, 260, 290, 292, 401, 464, 552
(0.75, 0.83, 1.65)

High Pressure
011, 015, 017, 018, 060, 075, 076, 079, 131, 166, 204, 225, 276, 323
336, 346, 418, 428, 445, 450, 458, 471, 484, 506
(3.48, 3.25, 5.65)

Magnetic Fields
008, 015, 020, 048, 049, 053, 072, 074, 075, 076, 120, 125, 157, 174
225, 226, 236, 323, 391, 392, 414, 416, 504
(2.85, 3.56, 5.41)

Radiation: Electrons
078, 122, 126, 143, 158, 263, 301, 317, 388, 435, 475
(1.51, 1.71, 2.59)

Radiation: Gamma Ray and Photons
017, 051, 053, 057, 061, 159, 192, 216, 226, 236, 317, 325, 368, 404
418, 512
(2.14, 3.10, 3.76)

Radiation: Ions
061, 218, 222, 226, 238, 239, 263, 277, 304, 321, 324, 388, 435, 481
(2.14, 3.45, 3.29)

Radiation: Neutrons
004, 056, 057, 128, 172, 200, 216, 218, 226, 236, 263, 321, 388, 410
432, 486
(1.95, 2.88, 3.76)
Radiation: Theory (use Theory: Defects and Radiation Effects in the Techniques index)
042, 200, 263, 430
(0.66, 1.16, 0.94)

Temperatures: Extremely High (above 1200degK)
003, 006, 010, 011, 021, 022, 040, 041, 047, 079, 115, 151, 154, 155
157, 219, 229, 231, 242, 260, 290, 292, 318, 336, 346, 383, 397, 411
412, 418, 445, 471, 486, 498
(5.55, 6.94, 8.00)

Temperatures: Cryogenic (below 77degK)
008, 011, 015, 020, 047, 048, 049, 050, 052, 056, 057, 059, 072, 075
076, 077, 078, 079, 081, 112, 120, 122, 123, 128, 129, 130, 156, 158
161, 164, 166, 174, 175, 206, 225, 226, 236, 302, 315, 322, 323, 352
369, 373, 390, 392, 403, 414, 418, 494
(7.39, 8.57, 11.76)

Vacuum: High (better than 10**9 Torr)
010, 014, 049, 050, 051, 052, 053, 061, 079, 124, 127, 176, 192, 237
238, 279, 355, 371, 381, 431, 503
(3.46, 4.32, 4.94)
MAJOR FACILITIES: OPERATIONS

Pulsed Neutron Sources (Operations)
046, 203
(0.47, 4.88, 0.47)

Steady State Neutron Sources (Operations)
082
(0.24, 7.42, 0.24)

Synchrotron Radiation Sources (Operations)
083, 298
(0.47, 8.89, 0.47)