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Materials Sciences Programs

Fiscal Year 1985

U.S. Department of Energy
Office of Energy Research
Office of Basic Energy Sciences
Division of Materials Sciences
Washington, D.C. 20545

FOREWORD

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 1985 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. Following that page is a list of the winners of the 1985 Materials Sciences Research Competition, a contest among the major laboratories within the three categories named.

Louis C. Ianniello, Director
Division of Materials Sciences
Office of Basic Energy Sciences

RECENT DIVISION SPONSORED PUBLICATIONS

Topical and Workshop Reports[a]

- Micromechanisms of Fracture (1985)[b]
- Polymer Research at Synchrotron Radiation Sources (1985)[a]
- Bonding and Adhesion at Interfaces (1985)
- Corrosion-Resistant Scales in Advanced Coal Combustion Systems (1985)
- Novel Methods for Materials Synthesis (1984)[c]
- Theory and Computer Simulation of Materials Structures and Imperfections (1984)[b]
- Materials Preparation and Characterization Capabilities (1983)
- Critical and Strategic Materials (1983)
- Coatings and Surface Modifications (1983)[c]
- High Pressure Science and Technology (1982)
- Scientific Needs of the Technology of Nuclear Waste Containment (1982)
- Radiation Effects (1981)
- Condensed Matter Theory and the Role of Computation (1981)
- Research Opportunities in New Energy-Related Materials (1981)[c]
- Aqueous Corrosion Problems in Energy Systems (1981)[c]
- High Temperature Corrosion in Energy Systems (1981)[c]
- Basic Research Needs and Opportunities on Interfaces in Solar Materials (1981)[c]
- Basic Research Needs on High Temperature Ceramics for Energy Applications (1980)[c]

Summary Research Bulletins (of Work in Progress)[a]

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

Description of Research Facilities, Plans, and Associated Programs

- Centers for Collaborative Research[a]
- Materials Sciences Division - Long Range Plan (1984)[a]
- Progress of the Office of Energy Research (1985)[a]

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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.

Winners of the 1985

Materials Sciences Research Competition
Within the DOE Laboratories

Category	Winners
Metallurgy and Ceramics:	
o Outstanding Scientific Accomplishment	T. A. Michalske, B. C. Bunker, G. A. Fisk, M. L. Knotek, and D. M. Haaland, SNL/A, "Stress Corrosion Cracking of Ceramics"
o Sustained Outstanding Research	R. M. Biefeld, L. R. Dawson, I. J. Fritz, G. C. Osbourn, P. L. Gourley, and D. R. Myers, SNL/A, "Strained Layer Superlattices (SLSs)"
o Significant Implication for Energy Technology	D. M. Follstaedt, J. A. Knapp, L. E. Pope, and S. T. Picraux, SNL/A, "Amorphization and Improved Friction and Wear of Steels by Implantation of Ti and C"
Solid State Physics	
o Outstanding Scientific Accomplishment	D. Gibbs, D. E. Moncton, J. Bohr, and K. L. D'Amico, BNL, "Synchrotron X-ray Scattering Studies of the Magnetic Structure of Holmium"
o Sustained Outstanding Research	K. G. Lynn, BNL, "Solid State Physics"
o Significant Implication for Energy Technology	B. R. Appleton, C. W. White, and O. E. Schow III, ORNL, "Surface Modification of Materials by Ion Beam Processing"
Materials Chemistry	
o Outstanding Scientific Accomplishment	J. M. Williams, K. D. Carlson, A. J. Schultz, M. A. Beno, H. W. Wang, and G. W. Crabtree, ANL, "Ambient Pressure Sulfur-Based Organic Superconductors: Synthesis, Structure, and Design"
o Sustained Outstanding Research	H. G. Drickamer, Univ. of Illinois, "The Pressure Tuning of Electronic Energy Levels"

ORGANIZATION OF THE DEPARTMENT OF ENERGY

Department of Energy

Secretary
Deputy
Under Secretary

Office of Energy Research

Assistant Secretaries

- Nuclear Energy
- Defense Programs
- Policy, Safety, and Environment
- Fossil Energy
- International Affairs & Energy Emergencies
- Management & Administration
- Congressional, Intergovernmental & Public Affairs

- Federal Energy Regulatory Commission
- Economic Regulatory Administration
- Energy Information Administration
- Conservation
- Renewable Energy

Office of Energy Research

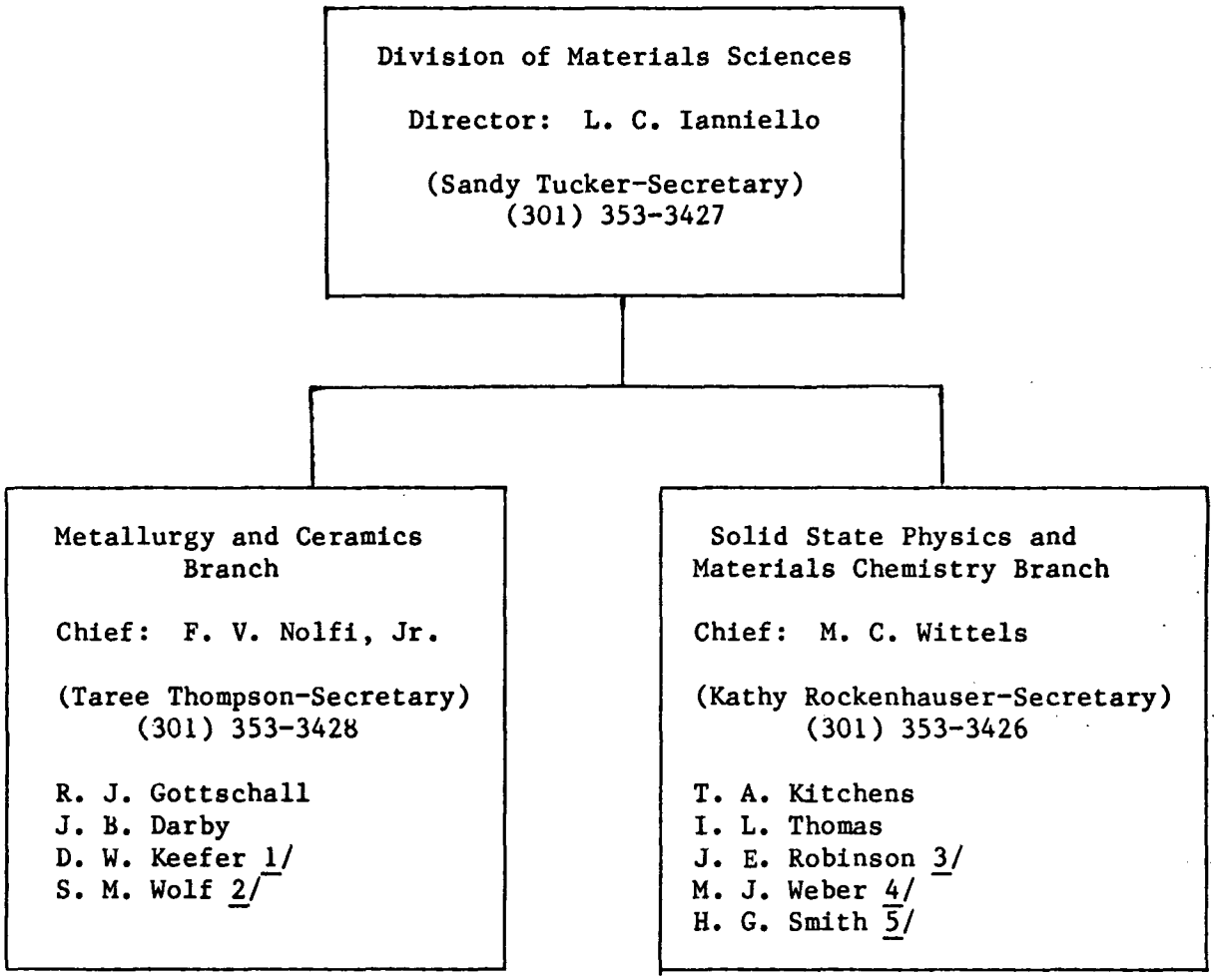
Director
Deputy

Associate Directors

1. Field Operations Management
2. Program Analysis
3. Fusion Energy (Magnetic)
4. High Energy & Nuclear Physics
5. Health & Environmental Research
6. Basic Energy Sciences
   - Materials Sciences
   - Chemical Sciences
   - Engineering & Geosciences
   - Advanced Energy Projects
   - Biological Energy Research
   - Carbon Dioxide Research

- Management
- Special Programs (Small Business Innovation Research)
- Scientific Computing
- Science & Technology Affairs

OFFICE OF BASIC ENERGY SCIENCES
Division of Materials Sciences Structure



Notes: 1/ On Detail from Idaho National Engineering Laboratory starting 10/85
2/ Now with the National Materials Advisory Board
3/ On Detail from Argonne National Laboratory starting 10/85
4/ Returned to Lawrence Livermore National Laboratory 9/85
5/ Returned to Oak Ridge National Laboratory 7/85

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 1985 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 1985 summary report was coordinated by T. A. Kitchens. Though the effort required time by every member of the Division, most of the work was done by Mrs. S. Tucker. This year the Summary was done "by the computer." This could not have been accomplished without the competent professional assistance of Mrs. K. Roskin, 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 although specific projects were concluded and others initiated this fiscal year.

AMES LABORATORY
Iowa State University
Ames, IA 50011

Metallurgy and Ceramics - 01 -

D. T. Peterson - Phone (FTS) 865-4446 or (515) 294-4446

001. MATERIALS SCIENCE OF INTERFACES

A. J. Bevolo, L. M. Seaverson
Phone: (515) 294-5414

$224,000 01-1

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 (350) 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.

002. NONEQUILIBRIUM MATERIALS

S. J. Poon, A. J. Drehman
Phone: (515) 294-4736

$283,000 01-1

Research on metallic glasses, metastable crystalline phases and extremely fine microstructural alloys. Ultra high vacuum melt spinning apparatus processes reactive metals without contamination. A directional solidification apparatus was modified to achieve extremely large undercooling and solidification rates. High speed planar solidification of eutectic Pb-Cd is being studied. Micro- structural study and superconductivity of metallic glasses and of rapidly crystallized solids. Future work will include the investigation of a wide range of metallic alloys.

003. SURFACES AND SOLIDIFICATION

R. K. Trivedi, J. T. Mason
Phone: (515) 294-5869

$228,000 01-1

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)

004. MICROSTRUCTURAL CONTROL IN METALS

J. D. Verhoeven, A. R. Pelton, E. D. Gibson, F. C. Laabs
Phone: (515) 294-9471

$325,000 01-1

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_3Sn and Nb_3Ga. Directional solidification studies on segregation and morphology in grey, nodular, and white cast iron. Evaluation of micro- structural changes in the austempering of nodular cast irons. Microstructure evolution under solidificaiton conditions typical of welding processes. Solidification processing of $(Dy,Tb)Fe_2$ magnetostrictive alloys.

005. MECHANICAL METALLURGY

W. A. Spitzig, J. Kameda, J. Kasichainula
Phone: (515) 294-5082

$530,000 01-2

Effects of hydrogen on crack initiation in refractory alloys under uniaxial and cyclic loading conditions. Investigation of hydrogen diffusion in vanadium-base alloys by internal friction. Hydrogen-induced brittle cracking in low 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.

006. STRUCTURE AND PROPERTY RELATIONS IN METALS

J. F. Smith
Phone: (515) 294-5083

$79,000 01-3

Thermodynamic functions in Y-Fe, Y-Co, and Y-Ni systems from electromotive force measurements. Computer analysis of thermodynamic data for the prediction of stable and metastable phase equilibria, metallic glass formation, and control of microstructures. Ultrasonic measurements of stress and texture in solids.

AMES LABORATORY (continued)

007. TRANSPORT STUDIES

O. N. Carlson
Phone: (515) 294-2375

$174,000 01-3

Study of fast diffusion and electrotransport of iron, cobalt and nickel in scandium and thorium. Determination of activation energies, mechanism and defect responsible for fast diffusion. Thermotransport and diffusion of interstitial solutes in vanadium-titanium and vanadium-niobium alloys. Determination of solid solubility of interstial solutes in vanadium.

008. HYDROGEN IN METALLIC SOLIDS

D. T. Peterson
Phone: (515) 294-6585

$236,000 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.

009. RARE EARTH MATERIALS

K. A. Gschneidner Jr., S. K. Dhar, P. Manfrinetti
Phone: (515) 294-2272

$231,000 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_3In 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.

AMES LABORATORY (continued)

010. NDE MEASUREMENT TECHNIQUES

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

$500,000 01-5

Techniques to measure failure-related material properties to improve understanding of failure mechanisms and inspection reliability. Ultrasonic measurment of internal stresses. Ultrasonic scattering and harmonic generation studies of fatigue cracks to provide information about closure near crack tip and the influence of this on 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.

011. ADVANCED MATERIALS AND PROCESSES

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

$184,000 01-5

New process for high-purity vanadium. Development of melting procedures for preparing Cu-Nb, Cu-Ta and Cu-Mo alloys. Alternative processes for preparing rare earth-iron alloys and for producing oriented crystallites of magnetostrictive compounds. Processing of stoichiometric and non-stoichiometric materials by an inducively coupled plasma. Electrotransport and zone melting for maximum purification of rare earth and refractory metals. Processing of single crystals of congruent melting and peritectic materials by levitation zone melting, free-standing vertical zone melting, Bridgman, Czochralski and strain-anneal recrystallization. Above research being conducted in the Materials Preparation Center described in the Section-Collaborative Research Centers.

Solid State Physics - 02 -

B. N. Harmon - Phone (FTS) 865-7712 or (515) 294-7712

012. NEUTRON SCATTERING

W. A. Kamitakahara, J. Mizuki, C. Stassis, J. Zarestky
Phone: (FTS) 865-4224 or (515) 294-4224

$365,000 02-1

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 (ScH_x, LaH_x), dynamics and phase transitions of alkali-graphite intercalation compounds, electronic structure and phonon spectra of mixed valence compounds ($CePd_3$, α-Ce, $YbAl_{12}$), relation of electron-phonon interaction to superconductivity (La, $LaSn_3$). High pressure studies (α-Ce, La). Study of the magnetic properties of heavy fermion superconductors ($CeCu_2Si_2$, UPt_3, UBe_{13}).

AMES LABORATORY (continued)

013. SEMICONDUCTOR PHYSICS

H. R. Shanks
Phone: (FTS) 865-6816 or (515) 294-6816
$225,000 02-2

Preparation and characterization of thin films, rf sputter desposition 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, photo-deflection and IR absorption spectroscopy. Measurements of gap state densities using DLTS, SCLC, and C-V on Schottky barriers.

014. SUPERCONDUCTIVITY

D. K. Finnemore, J. R. Ostenson, E. L. Wolf, T. P. Chen
Phone: (FTS) 865-3455 or (515) 294-3455
$445,000 02-2

Point contact Josephson effect in heavy fermion superconductors UBe_{13}, $CeCu_2Si_2$. Electron tunneling spectroscopy and surface physics studies of strong coupled transition metal superconductors. Proximity electron tunneling spectroscopy (PETS) of the electron-phonon spectrum $\alpha^2F(\omega)$. 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.

015. OPTICAL AND SPECTROSCOPIC PROPERTIES OF SOLIDS AND LIQUIDS

D. W. Lynch, C. G. Olson
Phone: (FTS) 865-3476 or (515) 294-3476
$305,000 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., $CeSn_3$) heavy Fermion systems, e.g., UPt_3, 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.

AMES LABORATORY (continued)

016. NEW MATERIALS AND PHASES

R. Shelton, C. A. Swenson, R. G. Barnes, M. S. Anderson,
P. Klavins, D. R. Torgeson
Phone: (FTS) 865-5435 or (515) 294-5435

$535,000 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 characterizaion of hydrogenated amorphous Si, Ge, SiC, and GeC films.

017. MATERIALS FOR HYDROGEN STORAGE

R. G. Barnes, A. Bevolo, O. Buck, J. D. Corbett, K. A. Gschneidner,
K.-M. Ho, D. T. Peterson, C. Stassis
Phone: (FTS) 865-4754 or (515) 294-4754 (515) 294-1560

$180,000 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. Insterstitial 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.

AMES LABORATORY (continued)

018. X-RAY DIFFRACTION PHYSICS

J.-L. Staudenmann, D. S. Robinson
Phone: (FTS) 865-3585 or (515) 295-3585 or 294-9614

$240,000 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 V_3Si and Fe-Ni-C in the vicinity of the martensitic phase transition. Active participation in the MATRIX PRT beam line at NSLS.

019. ELECTRONIC AND MAGNETIC PROPERTIES

B. N. Harmon, K.-M. Ho, M. Luban, D. Misemer, C. Soukoulis, J. Zhu
Phone: (FTS) 865-7712 or (515) 294-7712

$415,000 02-3

Theoretical studies of bulk and lattice dynamical properties of materials using first principles total energy calculation. Anharmonic interaction, lattice instabilities, phase transformation, electron-phonon interaction, and superconductivity. Equations of state (pressure and temperature). Hydrogen-metal interactions. Electron localization in disordered materials. Magnetism in spin glasses and ternary compounds. Electronic structure of rare earth compounds and transition metal sulfides and hydrides. Theory of amorphous semiconductor, and nuclear magnetic ordering in metals.

020. OPTICAL AND SURFACE PHYSICS THEORY

R. Fuchs, K.-M. Ho
Phone: (FTS) 865-3675 or (515) 294-3675

$165,000 02-3

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).

AMES LABORATORY (continued)

021. SUPERCONDUCTIVITY THEORY

J. R. Clem, V. G. Kogan
Phone: (FTS) 865-4223 or (515) 294-4223
$130,000 02-3

Electrodynamic behavior of current-carrying superconductors containing magnetic flux. Flux-line cutting and flux pinning in arrays of nonparallel vortices. Superconducting magnetic shielding. Critical fields and critical currents of proximity-coupled superconducting-normal (SN) multilayers and composites. Properties of Josephson and SNS junction arrays. 1/f noise and sensitivity to trapped magnetic flux in SQUIDs.

022. SYNTHESIS AND CHARACTERIZATION OF NEW MATERIALS

J. D. Corbett, R. E. McCarley, R. A. Jacobson, B. J. Helland
Phone: (515) 294-3086
$520,000 03-1

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-ZrI_4-ZrO_2, 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.

AMES LABORATORY (continued)

023. CERAMIC MATERIALS

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

$480,000 03-2

Synthesis of silicon-nitrogen polymers. Study of controlled thermal decomposition 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 decomposition 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 monodisperse powders in ceramics and catalysis. Studies of nucleation, growth, and agglomeration phenomena for control of precipitation and film deposition. Theoretical studies include DLVO theory for particle-particle interactions, coagulation and population balance equations for agglomeration kinetics. Investigation of reaction mechanisms and kinetics for high temperature reactions in the carbochlorination and carbonitrification processes to produce non-oxide ceramics.

024. HIGH TEMPERATURE CHEMISTRY OF REFRACTORY MATERIALS

H. F. Franzen
Phone: (515) 294-5773

$120,000 03-3

Study of refractory and corrosion-resistant materials such as transition metal aluminides (Zr-Al, Ta-Al), phosphides and sulfides by both experimental and theoretical techniques to understand the relationships among crystal structure, chemical bonding, and electronic structure as they affect high temperature stability, phase equilibria, and order-disorder transitions. Experimental methods include X-ray and electron diffraction for structure analysis, computer automated simultaneous mass loss-mass spectrometry for high temperature vaporization reactions related to stability, and photoelectron spectroscopy for the electronic structure of solids. Electronic structure studies also include a program of band structure calculations.

AMES LABORATORY (continued)

025. ELECTRONIC AND MAGNETIC PROPERTIES

R. S. Hansen, K. G. Baikerikar, D. C. Johnson, P. A. Thiel
Phone: (515) 294-2770

$480,000 03-3

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 spectroscopies, ring-disk and modulated hydrodynamic voltammetry.

ARGONNE NATIONAL LABORATORY
9700 S. Cass Avenue
Argonne, IL 60439

Metallurgy and Ceramics - 01 -

F. Y. Fradin - Phone (FTS) 972-4925 or (312) 972-4925
H. Wiedersich - Phone (FTS) 972-5079 or (312) 972-5079

040. DEFECTS IN METALS

R. W. Siegel, R. Benedek, J. E. Robinson, L.C. Smedskjaer, T. Lu, R. Prasad
Phone: (312) 972-4963

$804,000 01-3

Research program concerned with the atomic and electronic structure of defects in metals and alloys and the relationship between these and defect interactions, the properties of alloy phases, and the nature of phase transformations in alloy systems. The research involves investigations of defect properties and atomic and electronic structure in a variety of 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, resistometry, and transmission electron microscopy, and complementary electronic structure calculations.

041. DEFECTS IN CERAMICS

N. L. Peterson, K. L. Merkle, J. N. Mundy, J. L. Routbort, D. Wolf
Phone: (312) 972-4955

$941,000 01-3

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. Demixing of multicomponent oxides under oxygen potential gradients. Computer-assisted modeling of atomic transport in oxides. Effect of nonstoichiometry and defect clustering on mechanical deformation of oxides. Preparation of single crystals and bicrystals of metal oxides.

ARGONNE NATIONAL LABORATORY (continued)

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, T. Hashimoto, J. Mansfield
Phone: (312) 972-5021

$1,357,000 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, A. Taylor, N. J. Zaluzec
Phone: (312) 972-4964

$1,167,000 01-4

Development and use of high-voltage and high-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 and ion-beam analysis. 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 implantations 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 (120 kV) instruments.

ARGONNE NATIONAL LABORATORY (continued)

044. OXIDATION STUDIES

N. L. Peterson, D. J. Baxter, W. E. King, K. Natesan, S. J. Rothman
Phone: (312) 972-4955

$755,000 01-5

Cation and anion transport processes in pure and doped proctective-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. Effect of B and stoichiometry on grain-boundary and lattice transport processes in Ni_3Al.

045. AMORPHOUS METALLIC ALLOYS

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

$470,000 01-5

Investigations of the synthesis of amorphous metallic materials by isothermal solid-state reactions at the interfaces of vapor-deposited multilayer films and mixed metal powders, by ion-beam mixing of multilayer films, and by displacement damage of intermetallic compounds by electron and ion beams. In-situ high-voltage electron microscopy studies of the morphology and kinetics of the crystalline-to-amorphous transformations. The effect of irradiation on diffusion, segregation, and crystallization of amorphous alloys. Investigations of the relationship between the atomic structure of amorphous alloys and their magnetic and superconducting properties. Synthesis of ultra-fine metallic powders. Materials characterization methods include X-ray diffraction, electron microscopy, electrical resistivity, Rutherford backscattering, AES, EELS, and EXAFS.

ARGONNE NATIONAL LABORATORY (continued)

Intense Pulsed Neutron Source Program

G. H. Lander - Phone (FTS) 972-5518 or (312) 972-5518

046. INTENSE PULSED NEUTRON SOURCE PROGRAM

G. H. Lander, B. S. Brown, J. M. Carpenter, C. W. Potts, A. W. Schulke, T. G. Worlton, R. K. Crawford, F. J. Rotella, M. H. Mueller, C. K. Loong
Phone: (312) 972-5518

$4,830,000 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 7 instruments which are regularly scheduled for users and 3 beam tubes which are assigned to special experiments. The facility has been run since 1982 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 150 outside visitors from universities and other institutions, were performed in the period October 1982-October 1984. 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, Exxon) 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

D. L. Price, T. O. Brun, J. E. Epperson, J. Faber, G. P. Felcher, J. D. Jorgensen, P. R. Roach, S. Susman, R. O. Hilleke
Phone: (312) 972-5475

$1,941,000 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, chalcogenide and oxide glasses, surface magnetism, alloy decomposition and mixing, nonstoichiometric oxides, ultralow-temperature diffraction, spectroscopy of hydrocarbons, atomic momentum distributions with deep inelastic scattering, rapid solidification of glasses, and fast ion transport in solids.

ARGONNE NATIONAL LABORATORY (continued)

048. CHEMICAL AND ELECTRONIC STRUCTURE

J. M. Williams, M. A. Beno, C. D. Carlson, A. J. Schultz,
H. H. Wang, R. J. Thorn, T. J. Emge, U. Geiser, P. C. W. Leung
Phone: (312) 972-3464

$928,000 02-1

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.

049. 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

$1,296,000 02-2

Experimental and theoretical investigations of the magnetic and superconducting properties of materials. Studies of ternary compounds including Chevrel phase and rare-earth rhodium boride materials. Electronic and transport studies of organic superconductors. Studies of the electronic properties of mixed valence, heavy fermion and other narrow-band materials containing rare-earth and actinide elements. Studies of amorphous superconductors. Soft X-ray synchrotron beam-line development. Experimental techniques include the de Haas-van Alphen effect, Mossbauer spectroscopy, transport and magnetic measurements, electron tunneling, EELS, NMR, EXAFS and XANES, heat capacity, materials preparation, and characterization.

ARGONNE NATIONAL LABORATORY (continued)

050. ELECTRONIC STRUCTURE AND BONDING

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

$1,229,000 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 ABO_4 compounds using heat capacity, EXAFS, Raman scattering and ultrasonic measurements. Theoretical studies of photoelectron spectra and bonding of ABO_4 and AB_2O_4 compounds. Development of molecular cluster code to calculate total energy of embedded oxide clusters. Formulation of the theory of EXAFS and XANES for heavy elements. Angle resolved photoemission spectroscopy and de Haas-van Alphen studies of the electronic band structure of actinide intermetallic +compounds. Magnetization and photoemission spectroscopy (UPS and SPS) studies of actinide intermetallic compounds to determine the electronic configuration and stability of 5f electron states.

051. MATERIALS PREPARATION AND CHARACTERIZATION AND FAST ION TRANSPORT IN SOLIDS

S. Susman, S. D. Bader, M. B. Brodsky, M. Grimsditch, Y. Lepetre, E. Moog
Phone: (312) 972-5470

$793,000 02-2

Research on the growth and physical properties obtained by thin film techniques--epitaxial films and sandwiches, metallic and insulating superlattices, amorphous metals, and superconductors. Preparation techniques include molecular beam epitaxy, evaporation, and sputter deposition. Materials characterization methods include X-ray and neutron scattering, low- and high-energy electron diffraction, and electron microscopy 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. Theory of interface and growth phenomena.

ARGONNE NATIONAL LABORATORY (continued)

052. SYNCHROTRON RADIATION STUDIES

G. K. Shenoy, A. J. Arko, S. D. Bader, G. S. Knapp, A. R. Krauss, D. Y. Smith, M. G. Strauss, B. W. Veal Jr., C. E. Young
Phone: (312) 972-5537

$516,000 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.

053. CONDENSED MATTER THEORY

M. B. Brodsky, L. Guttman, R. Kalia, D. D. Koelling, A. Rahman, D. Y. Smith, P. Vashishta, K. Lee, M. Norman, M. Schneider, O. T. Valls
Phone: (312) 972-5016

$957,000 02-3

Condensed matter theory in statistical physics, electronic band structure, many-body effects, amorphous materials, and the defect solid state. Molecular-dynamics modeling of solvated electrons, defect mediated phase transitions, and multicritical behavior. Electronic structure calculations of narrow-band metal and alloy systems. Simulation of quantum systems by Monte Carlo methods. Optical and X-ray properties of solids. Superconductivity of heavy fermion superconductors. Spatial and electronic structure of covalent glasses. Transport in ionic conductors. Systems studied include molten salts, model surfaces and interfaces, ternary superconductors, rare earth and actinide compounds, electron-hole complexes, multilayers, and SiO_2 and chalcogenide glasses.

ARGONNE NATIONAL LABORATORY (continued)

054. ULTRA-HIGH FIELD SUPERCONDUCTORS

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

$262,000 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 and TEM. Coating of sputtered NbN films with copper stabilizer. Coating of both sides of tapes. Technique development for fabrication of continuous tapes and/or wires suitable for winding ultra-high field superconducting magnets.

Materials Chemistry - 03 -

F. Y. Fradin - Phone (FTS) 972-4925 or (312) 972-4925
D. M. Gruen - Phone (FTS) 972-3513 or (312) 972-3513

055. 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

$563,000 03-2

Experimental and theoretical investigations of important thermodynamic and structural properties of ordered and associated solutions, amorphous (metastable) materials, and strategic minerals. 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 Mossbauer spectroscopy, small angle neutron scattering, and inelastic neutron scattering are used to obtain data relating to valence states, ordering and clustering of atoms and ions in solution. The extension of our theories and concepts for pyrometallurgy will be explored. Electronic absorption spectroscopy, proton activation, X-ray diffraction, and cyclic voltammetry are used to explore the dissolution of metal compounds in domestic minerals and in industrial waste.

ARGONNE NATIONAL LABORATORY (continued)

056. INTERFACIAL MATERIALS CHEMISTRY

D. M. Gruen, V. A. Maroni, L. A. Curtiss, L. Iton, S. A. Johnson, C. A. Melendres, M. H. Mendelsohn, M. J. Pellin, M.-K. Ahn
Phone: (312) 972-3513

$334,000 03-2

Complementary fundamental research activities that focus on the structural and catalytic properties of macromolecular systems, including zeolites, metal atom clusters, and macrocyclic ligands. Studies of new aluminoferrisilicate zeolites having ZSM-5 and Offretite-like structures using electron paramagnetic resonance, nuclear magnetic resonance, Mossbauer, and infrared spectroscopies, as well as by high-voltage electron microscopy, and neutron inelastic scattering spectroscopy, 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, and excited state absorption spectroscopy 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 metal-water, polynuclear metal cluster, and interacting metal cluster-water species that yield incisive knowledge of adsorbate-substrate interactions on a molecular level. Spectroscopic (Raman, infrared, and electronic absorption) and electrochemical investigations that (1) probe the structural and bonding properties of macrocyclic organic ligands on electroactive surfaces, and (2) provide information on the mechanisms and rates of electron-transfer processes and electrocatalytic reactions.

ARGONNE NATIONAL LABORATORY (continued)

057. AQUEOUS CORROSION

D. M. Gruen, V. A. Maroni, L. A. Curtiss, C. A. Melendres, Z. Nagy, M. J. Pellin, R. M. Yonco, B. Biwer, J. McMahon
Phone: (312) 972-3513

$581,000 03-2

Basic research aimed at elucidating fundamental aspects of aqueous corrosion with emphasis on mechanisms responsible for stress corrosion cracking of iron and iron-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 corrodent metal-electrolyte interfaces and concurrent research directed towards testing corrosion models. Development of novel methods to simulate SCC crack tip and crevice environments and to elucidate the chemistry of these environments. 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 studies of corrosion-related charge transfer processes supported by parallel electrochemical measurements.

058. PARTICLE-SURFACE INTERACTION CHEMISTRY AND CATALYSIS

D. M. Gruen, W. F. Calaway, A. R. Krauss, G. J. Lamich, M. J. Pellin, M. W. Schauer, E. L. Schweitzer, C. E. Young
Phone: (312) 972-3513

$1,196,000 03-3

Surface analysis by resonance ionization of sputtered atoms (SARISA) using pico-coulomb ion fluences combined with direct 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.

BROOKHAVEN NATIONAL LABORATORY
Upton, NY 11973

Metallurgy and Ceramics - 01 -

A. N. Goland - Phone (FTS) 666-3819 or (516) 282-3819
M. Suenaga - Phone (FTS) 666-3518 or (516) 282-3518

070. BASIC PROPERTIES OF AMORPHOUS SEMICONDUCTING MATERIALS

P. E. Vanier, R. R. Corderman, F. J. Kampas
Phone: (FTS) 666-3535 or (516) 282-3535
$230,000 01-1

Investigations of the growth, structure, and properties of plasma-deposited thin-film amorphous semiconductors. Studies by optical and mass spectroscopy of processes in the plasma and their relation to film growth and defect formation. Studies of film structure and morphology by electron and optical microscopy, positron annihilation, and EXAFS. Studies of chemical bonding by infrared absorption and electron spin resonance. Measurement of photoelectronic properties and their correlation with structural and bonding characteristics.

071. MECHANISMS OF METAL-ENVIRONMENT INTERACTIONS

H. S. Isaacs, K. Sieradzki, J. S. Kim
Phone: (FTS) 666-4516 or (516) 282-4516
$420,000 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, S. Heald, T. Kuroda
Phone: (FTS) 666-3517 or (516) 282-3517
$570,000 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.

BROOKHAVEN NATIONAL LABORATORY (continued)

073. PHYSICAL PROPERTIES OF METAL-INTERSTITIAL SYSTEMS

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

$500,000 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. PROPERTIES OF DEFECTS IN MATERIALS

C. L. Snead Jr.
Phone: (FTS) 666-3502 or (516) 282-3502

$230,000 01-4

Effects of different types of irradiation on critical properties of type-II superconductors, electron, reactor neutron, 14-MeV neutron, 17-MeV, 800-MeV and 30 GeV proton irradiations, Nb-Ti, and A15 superconductors, defect and microstructure changes in irradiated materials, application of positron annihilation to defect studies: irradiation-induced defects and gases in metals. Mechanical properties of various materials using internal friction and dynamical Young's modulus techniques, study of hydrogen in metals and martensitic transformations.

BROOKHAVEN NATIONAL LABORATORY (continued)

Department of Chemistry - 02 -

A. P. Wolf - Phone (FTS) 666-4397 or (516) 282-4376

075. NEUTRON SCATTERING

L. M. Corliss, J. M. Hastings, R. Thomas
Phone: (FTS)-666-4376 or (516) 282-4376
$445,000 02-1

Neutron scattering studies of the statistical mechanics of phase transitions, the dynamical properties 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 -

V. J. Emery - Phone (FTS) 666-3765 or (516) 282-3765

076. MAGNETIC AND STRUCTURAL PHASE TRANSITIONS

S. M. Shapiro, J. D. Axe, P. Boni, H. Grimm, J. Martinez, J. P. Wicksted, H. Yoshizawa
Phone: (FTS) 666-3822 or (516) 282-3822
$1,260,000 02-1

Neutron scattering studies of the structure and dynamics of phase transitions. Random magnetic systems, magnetic superconductors, low dimensional charge density waves, incommensurate systems and soft modes in solids.

077. ELEMENTARY EXCITATIONS AND NEW TECHNIQUES

G. Shirane, M. Chen, A. Goldman, A. Heidemann, C. F. Majkrzak, L. Passell, J. P. Wicksted, Y. J. Uemura
Phone: (FTS) 666-3732 or (516) 282-3732
$1,550,000 02-1

Neutron scattering studies of low-lying excitations in solids and overlayer films, electron-phonon interactions in metals and lattice dynamics of metal hydride systems. Development of efficient neutron polarizers and new devices for beam modulation.

BROOKHAVEN NATIONAL LABORATORY (continued)

078. EXPERIMENTAL RESEARCH - X-RAY SCATTERING

J. D. Axe, J. Bohr, K. D'Amico, L. D. Gibbs, D. E. Moncton, D. Osterman
Phone: (FTS) 666-3821 or (516) 282-3821
$1,005,000 02-2

Structural and dynamical properties of condensed matter systems, studied by X-ray and neutron scattering, phase transitions and new states of matter particularly in two-dimensional (2D) systems: 2D melting, commensurate-incommensurate transitions, reconstruction, and molecular orientation transitions. Extension to single crystal surfaces under ultra high vacuum conditions is in progress, studies of magnetic and magnetoelastic X-ray scattering including the use of X-ray polarization analysis, study of the structure of atomic microclusters produced in nozzle beams, research and development studies of synchrotron instrumentation for NSLS experiments.

079. LOW ENERGY - PARTICLE INVESTIGATIONS OF SOLIDS

K. G. Lynn, D. Chen (CCNY), W. Frieze, D. Gidley (Bell Labs), C. Lewis (DAS), R. Mayer, B. Nielsen, L. Roellig (CCNY), M. Weber (CCNY), C. Zhang
Phone: (FTS) 666-3710 or (516) 282-3710
$970,000 02-2

Investigations of perfect and imperfect solids and their surfaces by newly developed experimental methods, use of both magnetically and electrostatically focussed variable energy positron beams coupled with standard surface analysis tools (Auger Electron Spectroscopy, Low Energy Electron Diffraction, Photoemission, Thermal Desorption Spectroscopy), high resolution positron energy loss measurements of adsorbed molecules on metal surfaces, surface state lifetimes, positron diffusion lengths, positron work functions, positronium formation with measurement of its emitted energy distribution, metal-metal and metal-insulator interfaces, ion implanted and laser annealed semiconductors, use of recently developed muSR channel at AGS.

080. ADVANCED MATERIALS SYNTHESIS AND CHARACTERIZATION

D. E. Cox, K. G. Lynn, A. Moodenbaugh
Phone: (FTS) 666-3818/3870 or (516) 282-3818/3870
$490,000 02-2

Preparation and characterization of inorganic materials by high temperature, sputtering and solution techniques, crystal orientation, development and application of profile methods for structural analysis of neutron and X-ray powder diffraction data, application of synchrotron radiation to high resolution powder diffractometry.

BROOKHAVEN NATIONAL LABORATORY (continued)

081. THEORETICAL RESEARCH

P. Bak, S. Coppersmith, J. Davenport, G. J. Dienes, V. J. Emery, Y. Shapir, R. M. Sternheimer, G. Vineyard, R. E. Watson, M. Weinert
Phone: (FTS) 666-3798 or (516) 282-3798
$700,000 02-3

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, electronic structure of metals and alloys, X-ray and neutron scattering, properties of disordered materials and crystal defect physics, high pressure, high temperature properties of solids.

082. SURFACE PHYSICS RESEARCH

M. Strongin, S. Hulbert, P. D. Johnson, S. Raaen, M. Shek
Phone: (FTS) 666-3763 or (516) 282-3763
$900,000 02-5

Synchrotron Radiation as a technique to study the geometrical and electronic properties of surfaces and interfaces. Special emphasis has also been given to the development of new spectroscopies such as inverse photoemission and the construction of an undulator beam line at the NSLS to enable experiments on spin polarized photoemission. 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 and clean metal surfaces, and hydrogen on metal surfaces, also 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 transitons in adsorbate layers on metal surfaces. In particular, studies of phase transitions of Xe layers on metal surfaces: e) properties of ion implanted surfaces, f) studies of metal clusters in rare gases and in organic solids, g) studies of oxidation and other chemical reactions at low temperatures.

BROOKHAVEN NATIONAL LABORATORY (continued)

High Flux Beam Reactor - 02 -

G. C. Kinne - Phone (FTS) 666-4061 or (516) 282-4061

083. EXPERIMENTAL RESEARCH-HIGH FLUX BEAM REACTOR - OPERATIONS

G. C. Kinne, D. C. Rorer, M. H. Brooks, R. C. Karol, D. G. Pitcher, O. Jacobi, S. Protter, L. Junker, P. Tichler, J. Detweiler, W. Brynda
Phone: (FTS) 666-4061 or (516) 282-4061

$8,065,000 02-1

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

084. NATIONAL SYNCHROTRON LIGHT SOURCE, OPERATIONS AND DEVELOPMENT

M. Knotek, M. Barton, K. Batchelor, R. Blumberg, J. Galayda, J. Godel, J. Hastings, R. Heese, H. Hsieh, R. Klaffky, S. Krinsky, A. Luccio, C. Pellegrini, W. Thomlinson, A. van Steenbergen, G. Vignola, G. Williams
Phone: (FTS) 666-4966 or (516) 282-4966

$9,705,000 02-2

Support of 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 beamlines of the vacuum ultraviolet (VUV) and X-ray storage rings, NSLS encompasses the further improvement of the storage rings to achieve maximum brightness photon sources and the further development of the photon beamlines of the facility by means of new developments in high resolution photon optics, state-of-the-art monochromators, X-ray mirror systems, detectors and other necessary instrumentation. The NSLS storage rings will provide extremely bright photon sources, several orders of magnitude more intense in the VUV and X-ray regions than conventional sources. This facility is the first in this country to be designed expressly for generation and use of synchrotron radiation. An extensive research and development program is 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 effort also supports the construction of the beam lines and devices funded under the Phase II construction project.

IDAHO NATIONAL ENGINEERING LABORATORY
550 2nd Street
Idaho Falls, ID 83401

Materials Processing Branch - 01 -

J. F. Key - Phone (FTS) 583-8332 or (208) 526-8332

100. MATERIALS SCIENCE WELDING RESEARCH

J. F. Key, H. B. Smartt, M. E. McIlwain
Phone: (FTS) 583-8332 or (208) 526-8332

$380,000 01-5

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, high-speed X-radiography, optical and electron microscopy, calorimetry, and computer modeling. Technology transfer through American Welding Technology Applications Center.

UNIVERSITY OF ILLINOIS MRL
104 S. Goodwin Avenue
Urbana, IL 61801

Metallurgy and Ceramics - 01 -

H. K. Birnbaum - Phone (217) 333-4778 or (217) 333-1901

105. EFFECT OF FLUID FLOW ON LOCALIZED CORROSION

R. C. Alkire
Phone: (217) 333-0063

$70,000 01-1

Corrosion of passivating systems. Mechanisms of corrosion pit formation. Transport, kinetics and convective diffusion at localized corrosion sites. Erosion, cavitation, pitting, repassivation, and transient metal salt films. 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

$180,000 01-1

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

$180,000 01-1

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

$135,000 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_2 chalcopyrite systems.

UNIVERSITY OF ILLINOIS MRL (continued)

109. PROCESSING AND CHARACTERIZATION OF NOVEL AMORPHOUS MATERIALS AND SURFACES

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

$60,000 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 $Cu_xCr_{(1-x)}$ alloys.

110. MICROCHEMISTRY OF SOLIDS

C. A. Wert
Phone: (217) 333-1440

$70,000 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.

111. PROCESSING AND MICROSTRUCTURE OF COMPLEX CERAMIC SYSTEMS

A. Zangvil
Phone: (217) 333-6829

$120,000 01-1

Microstructure and microchemistry of SiC-AlN, SiC-BeO, SiC-BN and SiC. Effect of processing variables and additives on the structure and microchemistry of ceramic systems. Hydrogen effects in SiC. Role of chemistry in the formation of polytypes.

112. HYDROGEN BEHAVIOR IN BCC METALS

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

$125,000 01-2

Mobility of hydrogen and deuterium in b.c.c. 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.

UNIVERSITY OF ILLINOIS MRL (continued)

113. MICROMECHANICS AND MICROMECHANISMS OF FRACTURE

H. K. Birnbaum, C. J. Alstetter, F. A. Leckie, R. M. McMeeking, D. Socie, J. F. Stubbins, I. Robertson
Phone: (217) 333-1901

$565,000 01-2

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, Al_2O_3-ZrO_2, 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

D. Lazarus
Phone: (217) 333-0492

$65,000 01-2

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

$70,000 01-2

Deformation characteristics of diborides and non-stoichiometric monocarbides of IVb and Vb transition metals at extremely high temperatures. Dislocation properties, second phase precipitates, and their role in diffusion limited flow stress. Microchemical analysis of precipitates, grain boundaries and stacking faults by EELs.

UNIVERSITY OF ILLINOIS MRL (continued)

116. DEVITRIFICATION BEHAVIOR IN METAL-CONTAINING SILICATE AND BOROSILICATE GLASSES

H. Chen
Phone: (217) 333-7636

$65,000 01-3

Investigation of devitrification kinetics and associated microstructural and compositional changes in silicate and borosilicate-based glasses containing metal oxides using EXAFS, small and wide-angle X-ray scattering and SEM methods. Mechanisms of metal-silicide thin film formation. Kinetics of layer growth.

117. A BUILD-BLOCK APPROACH TO THE SYNTHESIS OF NEW INORGANIC MATERIALS

W. F. Klemperer
Phone: (217) 333-2995

$130,000 01-3

Low-temperature synthesis of oxide glasses and ceramics using step-wise synthesis. Polynuclear molecular building-blocks are assembled and then formed into solid materials using gel-solidification methods. $[Si_8O_{12}](OCH_3)_8$ molecular cages, and their linkage reactions are studied using optical and molecular spectroscopies.

118. DIELECTRIC SOLIDS

D. A. Payne
Phone: (217) 333-2937

$125,000 01-3

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

UNIVERSITY OF ILLINOIS MRL (continued)

119. MICROSTRUCTURE AND CRYSTALLIZATION IN NOVEL GLASSY SYSTEMS

S. H. Risbud
Phone: (217) 333-2885

$85,000 01-3

Glass synthesis and phase transformations in quasi-binary II-IV-V2 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) 333-0073

$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.

Solid State Physics - 02 -

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

121. LOW-TEMPERATURE STUDIES OF DEFECTS IN SOLIDS

A. C. Anderson
Phone: (217) 333-2866

$95,000 02-2

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 0.02-200 K.

UNIVERSITY OF ILLINOIS MRL (continued)

122. PHOTOEMISSION STUDIES OF THE ELECTRONIC STRUCTURE OF SURFACES AND INTERFACES

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

$145,000 02-2

Synchrotron radiation photoemission studies of electronic structure of semiconductor surfaces and interfaces prepared in-situ by molecular beam epitaxy, adsorption kinetics and catalysis on surfaces, properties of alloy surfaces.

123. HIGH-FIELD SUPERCONDUCTORS

D. M. Ginsberg
Phone: (217) 333-4356

$75,000 02-2

Investigation of high-field superconductors by preparation and detailed characterization of samples and by measurements of critical magnetic field, specific heat, Raman effect, magnetic susceptibility, neutron diffraction, and transport properties.

124. ULTRASONIC STUDIES OF THE STRUCTURE OF MATTER

A. V. Granato
Phone: (217) 333-2639

$125,000 02-2

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

125. PROPERTIES OF CRYSTALLINE CONDENSED GASES

R. O. Simmons, V. R. Pandharipande
Phone: (217) 333-3760 or (217) 333-8079

$200,000 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.

UNIVERSITY OF ILLINOIS MRL (continued)

126. NUCLEAR MAGNETIC RESONANCE IN SOLIDS

C. P. Slichter
Phone: (217) 333-3834

$225,000 02-2

Investigations of layered materials and one dimensional conductors with charge density waves, of platinum-alumina reforming hydrocarbon catalysts, and of spin glasses using nuclear magnetic resonance methods.

127. PHYSICAL PROPERTIES OF ORDERED AND DISORDERED SOLID SOLUTIONS

H. Zabel
Phone: (217) 333-2514

$155,000 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.

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

H. G. Drickamer
Phone: (217) 333-0025

$180,000 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.

129. EXCITON COLLECTION FROM ANTENNA SYSTEMS INTO ACCESSIBLE TRAPS

L. R. Faulkner
Phone: (217) 333-8306

$60,000 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.

LAWRENCE BERKELEY LABORATORY
1 Cyclotron Road
Berkeley, CA 94720

Materials and Molecular Research Division - 01 -

Norman E. Phillips - Phone (FTS) 451-6062 or (415) 486-6062

140. STRUCTURE AND PROPERTIES OF TRANSFORMATION INTERFACES

R. Gronsky
Phone: (FTS) 451-5674 or (415) 486-5674
$210,000 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
$620,000 01-1

Fundamental electron microscopic studies of the structure-chemistry-processing-property relationships. Specific tasks: a) ferrite-martensite steels for rod and wire: microstructure and processing, solute partitioning, fatigue (with Prof. R. Ritchie), wear. b) martensitic and bainitic steels: fundamental studies of phase transitions, relation to wear, grain boundary precipitation and effect of copper, processing for maximum toughness. c) electronic materials: structure of audio recording tape, piezoelectric materials, and rare-earth alloys.

142. SOLID-STATE PHASE TRANSFORMATION MECHANISMS

K. H. Westmacott
Phone: (FTS) 451-5663 or (415) 486-5663
$210,000 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.

LAWRENCE BERKELEY LABORATORY (continued)

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

$1,400,000 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 micromechanical 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

$110,000 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 to be observed at full magnification. In situ studies of nucleation and growth using solid electrolytes.

145. LOCAL ATOMIC CONFIGURATIONS IN SOLID SOLUTIONS

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

$140,000 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_3Pd and Ag_3Mg using electron microscopy. Short range order studies in Au_4Fe, Ni_4Mo and similar systems.

LAWRENCE BERKELEY LABORATORY (continued)

146. COLLABORATIVE RESEARCH BY TRANSMISSION ELECTRON MICROSCOPY

N. E. Phillips
Phone: (FTS) 451-6062 or (415) 486-6062
$50,000 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 with Materials and Molecular Research Division Investigators recommended for support by the NCEM Steering Committee.

147. THEORETICAL PROBLEMS IN ALLOY DESIGN

J. W. Morris Jr.
Phone: (FTS) 451-6482 or (415) 486-6482
$575,000 01-2

Multifaceted program of metallurgical research that is concerned with the science of alloy design. Current research includes work on the following alloy types: (1) high-strength, high-toughness ferritic steels, (2) carbon steels with exceptional formability, (3) high-strength, low-density aluminum-lithium alloys, (4) fatigue-resistant lead-tin solder contacts, (5) high-field superconducting wire. Each of these alloy design efforts is supported by fundamental research on the relevant structure-property and structure-processing relations.

148. MECHANICAL PROPERTIES OF CERAMICS

A. G. Evans
Phone: (415) 642-7347
$305,000 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.

LAWRENCE BERKELEY LABORATORY (continued)

149. ENVIRONMENTALLY AFFECTED CRACK GROWTH IN ENGINEERING MATERIALS

R. O. Ritchie
Phone: (FTS) 451-5798 or (415) 486-5798

$300,000 01-2

To examine, from continuum and micro-mechanistic points of view, the respective roles of mechanical, microstructural, and environmental factors involved in the subcritical monotonic and cyclic growth of flaws in engineering materials. Current emphasis is devoted to i) defining the role of microstructure on crack closure mechanisms and their effect on subsequent-near-threshold fatigue growth of long and short cracks in steels below 10^{-5}mm/cycle, and ii) the modeling of crack initiation and crack growth toughness for monotonic fracture by both cleavage and void coalescence. The aim of this work is to present mechanically derived guidelines for the development of both improved failure prediction and improved alloy design of fracture-critical materials.

150. INTERFACES AND CERAMIC MICROSTRUCTURES

J. A. Pask
Phone: (415) 642-3821

$10,000 01-3

Kinetics and mechanisms of solid-state reactions, nucleation and growth phenomena, and distribution of phases in multiphase ceramic systems whose principal phase constituents are within the Al_2O_3-SiO_2 system. Thermodynamic considerations of sintering with a liquid phase. Mechanisms of corrosion of ceramic materials. Thermodynamics and kinetics of electrochemical reactions at glass-metal interfaces.

151. HIGH-TEMPERATURE REACTIONS

A. W. Searcy
Phone: (FTS) 451-5900 or (415) 486-5900

$350,000 01-3

TEM characterization of the crystallinity, particle size, and pore dimensions of high-surface-area oxides. Experimental studies of $CaCO_3$ + TiO_2 = $CaTiO_3$ + CO_2 and the development of new thermodynamic models for complex solid solutions.

LAWRENCE BERKELEY LABORATORY (continued)

152. STRUCTURE-PROPERTY RELATIONSHIPS IN SEMICONDUCTOR MATERIALS

J. Washburn
Phone: (FTS) 451-6254 or (415) 486-6254
$350,000 01-3

Semiconductor/metal and semiconductor/insulator interfaces. Mechanism of the crystalline-to-amorphous transformation during ion damage in silicon and gallium arsenide, and an investigation of the mechanism of growth of thin-film layers on surfaces. High-resolution microscopy and computer simulation of images combined with complementary observations on the same specimens such as electron paramagnetic resonance, secondary ion mass spectroscopy, and optical or electrical measurements.

153. CHEMICAL PROPERTIES AND PROCESSING OF REFRACTORY CERAMICS

L. C. De_Jonghe
Phone: (FTS) 451-6138 or (415) 486-6138
$250,000 01-3

Structure of the interface between nickel and zirconia using analytical and high-resolution transmission electron microscopy. Ni/ZrO_2 cermets in as-fabricated and thermally cycled conditions. Interface bond strength and the residual stresses at the interface are examined by indentation techniques, and the onset of cracking at the interface during thermal cycling is detected by acoustic emission monitoring and related to interface microstructure and microchemistry.

154. STRUCTURE AND ELECTRICAL PROPERTIES OF COMPOSITE MATERIALS

R. H. Bragg
Phone: (415) 642-7393
$125,000 01-3

Studies to determine why soft carbons graphitize, i.e., become physically soft when heated above about 2000°C in inert atmosphere, whereas hard carbons do not, even when heated above 3000°C. Direct synthesis and related experimental studies of the carbon-hydrogen system are being performed.

LAWRENCE BERKELEY LABORATORY (continued)

155. HIGH-TEMPERATURE OXIDATION AND CORROSION OF MATERIALS

N. E. Phillips
Phone: (FTS) 451-6062 or (415) 486-6062

$95,000 01-3

Research on the mechanisms by which materials withstand high-temperature corrosion attack, and the development of protective scales. Factors of major significance include: the initial development of the protective scale, the transport of reactants in and through the scale, the scale structure, morphology, and growth mode, and the chemical integrity of the scale when exposed to corrosive sulfate deposits. Relationship of mechanisms of behavior to the thermodynamic, diffusional, structural, and compositional parameters of the metal oxides, sulfides, and other phases involved. Quantitative and predictive alloy corrosion models.

156. CERAMIC INTERFACES

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

$145,000 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, high-resolution TEM characterization of high-angle grain boundaries in lead to determine whether direct evidence exists for grain-boundary structure transformations, and theoretical modeling of the effect of concurrent grain-boundary migration and tracer self diffusion on apparent grain-boundary diffusivities.

157. ABRASIVE, EROSIVE, AND SLIDING WEAR OF MATERIALS

I. Finnie
Phone: (415) 642-1496

$110,000 01-5

Basic mechanisms of abrasive, erosive, and sliding wear for different classes of materials.

LAWRENCE BERKELEY LABORATORY (continued)

158. EROSION-CORROSION WEAR PROGRAM

N. E. Phillips
Phone: (FTS) 451-6062 or (415) 486-6062

$15,000 01-5

Development of a model for predicting erosion of ductile metals from analytical expressions that define the two-phase fluid flow of a gas-solid particle stream and equations that describe the platelet mechanism of erosion. Experimental studies of boundary-layer gas to protect the surface of coal reactors from high-temperature corrosion.

159. EROSION OF BRITTLE SOLIDS

A. G. Evans
Phone: (415) 642-7347

$130,000 01-5

Development of a fundamental understanding of the spalling erosion and strength degradation of brittle coatings and layers subject to thermal and mechanical (impact) loading. Principal research directions involve studies of damage created by mechanical and thermal loads, by impacting particles, and by thermal shock. Studies of residual stresses at and adhesion of coating interfaces.

160. FAR-INFRARED SPECTROSCOPY

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

$230,000 02-2

Improved infrared detectors, mixers, and spectrometers 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 50-500 μm wavelength range, improved fabrication techniques for bolometric detectors, a new class of far-infrared beam dividers, and production of tunable picosecond far-infrared pulses by difference frequency generation. Experiments include measurements of the infrared spectra of adsorbed molecules and of one-dimensional charge-density wave conductors, measurements of the infrared photoconductivity of impurities in semiconductors, and a test of the Planck theory of thermal radiation with unprecedented accuracy.

LAWRENCE BERKELEY LABORATORY (continued)

161. EXPERIMENTAL SOLID-STATE PHYSICS AND QUANTUM ELECTRONICS

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

$270,000 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, and phase transitions, surfaces and interfaces.

162. EXCITATIONS IN SOLIDS

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

$180,000 02-2

Studies of the onset of instabilities and pseudorandom behavior in solids. Systematic study of the chaotic dynamics of driven p-n junctions to reveal universal patterns: period-doubling bifurcations, onset of chaos, periodic windows, and intermittency. Spin-wave instabilities in ferrite spheres: period doubling, chaos, and intermittency, and they can be understood by a two-dimensional quadratic map. Spatial and temporal chaotic behavior is in electron-hole plasma-density waves in crystals of Ge: period-doubling route to chaos, periodic windows, and quasiperiodicity. These results have a bearing on devices of high technological importance.

163. TIME-RESOLVED SPECTROSCOPIES IN SOLIDS

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

$100,000 02-2

The main objective of this project is to utilize picosecond and sub-picosecond 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.

LAWRENCE BERKELEY LABORATORY (continued)

164. SUPERCONDUCTIVITY, SUPERCONDUCTING DEVICES, AND 1/F NOISE

J. Clarke
Phone: (415) 642-3069

$270,000 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.

165. THEORETICAL STUDIES OF THE ELECTRONIC PROPERTIES OF SOLID SURFACES

L. M. Falicov
Phone: 415-642-5993

$75,000 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).

LAWRENCE BERKELEY LABORATORY (continued)

166. THEORETICAL SOLID-STATE PHYSICS

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

$105,000 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.

167. SURFACE, CHEMISORPTION, AND THEORY OF SOLIDS

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

$50,000 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.

168. LOW-TEMPERATURE PROPERTIES OF MATERIALS

N. E. Phillips
Phone: (FTS) 451-6062, (415) 486-6062, or (415) 642-4855

$126,000 03-1

Research on low-temperature properties of materials and on methods of temperature measurement. Measurements on 3He in the Fermi-liquid region have established the correct values of parameters that are important to understanding superfluid states, on potassium, rubidium, and cesium to 0.1\K to test theoretical predictions of charge-density-wave effects, and on predicted phase boundary of the spin-glass phase. Specific future objectives: an extension of the 3He measurements to the superfluid phases, additional studies on spin glasses, and specific-heat measurements at pressures to 20\kbar on mixed-valence compounds.

LAWRENCE BERKELEY LABORATORY (continued)

169. ELECTROCHEMICAL PROCESSES

C. W. Tobias
Phone: (FTS) 451-5208 or (415) 486-5208
$117,000 03-1

Novel methods for reducing mass-transfer resistance in high-rate applications, including in electro-forming of metals, and in electroorganic synthesis. Transport rates and current distribution are measured over broad ranges of process variables, theoretical models are advanced for the interpretation of mechanisms. Nonaqueous ionizing solvents explored for potential use in ambient-temperature electrosynthesis processes, with emphasis on the separation, electrowinning, refining, and electroplating of reactive metals.

170. HIGH-TEMPERATURE THERMODYNAMICS

L. Brewer
Phone: (FTS) 451-5946 or (415) 486-5946
$164,000 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.

171. CHEMISTRY AND MATERIALS PROBLEMS IN ENERGY PRODUCTION TECHNOLOGIES

D. R. Olander
Phone: (415) 642-7055
$281,000 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 UO_2. 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.

LAWRENCE BERKELEY LABORATORY (continued)

172. ELECTROCHEMICAL PHASE BOUNDARIES

R. H. Muller
Phone: (FTS) 451-6079 or (415) 486-6079
$178,000 03-3

Development and use of new optical techniques and interpretation procedures of solid-liquid interfaces. The nature and the mechanism of formation of surface layers on metals are investigated while they are immersed in liquids, with sensitivity to fractional monolayer coverage of absorbed or reacted materials. Mass-transfer boundary layers are studied to determine the concentration of reacting species in the liquid immediately adjacent to the surface at which they react, and to judge the effectiveness of different measures taken to increase the rate and uniformity of electro-chemical reactions.

173. SOLID-STATE AND SURFACE REACTIONS

G. A. Somorjai
Phone: (415) 642-4053
$389,000 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.

174. NUCLEAR MAGNETIC RESONANCE

A. Pines
Phone: (FTS) 451-6097 or (415) 486-6097
$215,000 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 nuclear magnetic isotope separation. 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.

LAWRENCE BERKELEY LABORATORY (continued)

175. SYNTHESIS OF NOVEL SOLIDS

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

$20,000 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.

Accelerator and Fusion Research Division - 02 -

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

176. R&D FOR ADVANCED PHOTON SYSTEMS

M. R. Howells, D. T. Attwood, K. S. Halbach, K.-Je Kim
Phone: (FTS) 451-4949

$1,110,000 02-2

The synchrotron radiation community is now on the threshold of developing a new generation of X-ray facilities which will produce radiation which is extremely bright, powerful, and in some cases partially coherent. To realize these opportunities research and development is required to extend state-of-the-art technologies in two critical areas: (1) Many period permanent magnet structures (undulators and wigglers), (2) Photon (beam line) systems must be designed and constructed which are both efficient and phase space conserving under high thermal loading and high intensity conditions.
This program addresses design studies of next-generation undulators and the design and fabrication of high thermal-loading beamline hardware which will be tested under the most extreme conditions achievable on present facilities.

LAWRENCE BERKELEY LABORATORY (continued)

177. CENTER FOR X-RAY OPTICS

D. Attwood
Phone: (FTS) 451-4463 or (415) 486-4463

$1,150,000 02-2

Development of technologies required for the utilization of emerging sources of XUV radiation in application for science and industry. The Center has organized laboratories and collaborations which will lead 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. 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.

Center for Advanced Materials - 03 -

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

178. CAM CATALYSIS PROGRAM

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

$850,000 03-3

Synthesis, characterization, evaluation of new catalysts: synthetic zeolites and other microporous crystals, transition-metal compounds, transition-metal complex catalysis in novel matrices, catalytic reactions stimulated by plasma or laser excitation. Discovery of new, lower cost catalysts with increased selectivity and resistance to degradation in industrial conditions. Zeolite synthesis, characterization by high-resolution EM, extended X-ray fine structure, solid-state NMR, adsorption studies to relate synthesis with structure. Determination of structure and catalytic properties of carbides and nitrides of Group IV-VI transition metals and some Group VII silicides. Supported and bulk configurations. Synthesis of organometallic molecules anchored to organic and inorganic polymer surfaces. Evaluation of potentially unique catalytic properties e.g., as films on electrodes.

LAWRENCE BERKELEY LABORATORY (continued)

179. CAM ELECTRONIC MATERIALS PROGRAM

Eugene Haller
Phone: (415) 486-5294

$850,000 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, epitaxial films, 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 Czochralski and Bridgman furnaces. 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.

180. CAM ADVANCED INSTRUMENTATION FOR SURFACE SCIENCE PROGRAM

J. Clarke
Phone: (415) 642-3069

$400,000 02-5

Scanning tunneling microscope development focusing on achievement of atomic resolution, sample introduction and withdrawal from ultrahigh vacuum chamber without breaking vacuum, and computer control of microscope operation and data collection. Use of the instrument for study of surface reconstruction, location of absorbed atoms and molecules, the structure of as-grown semiconductors, and the effects of laser annealing. 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.

LAWRENCE BERKELEY LABORATORY (continued)

181. CAM ADVANCED STRUCTURAL CERAMICS

L. De Jonghe
Phone: (415) 486-6138

$350,000 01-1

Basic research effort on high-temperature structural ceramics focusing on microstructural heterogeneities: how they arise, affect mechanical properties of ceramics, and can be manipulated. Experimental and theoretical study of static and dynamic colloid behavior in relation to slip casting and injection molding, study of the development of microstructural heterogeneities arising at the particle level, establishment and verification of high-temperature creep-failure theories, and study of fundamental aspects of erosion and wear. Multiparticle interactions in concentrated colloids, incorporating surface chemistry, characterization by microscopy, chemical modification of powder surfaces and surface characterization, two-dimensional studies of multiparticle densification at the particle level, creep sintering, study of creep rupture by shear band cavitation at high temperatures.

182. CAM POLYMERS AND POLYMER COMPOSITES PROGRAM

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

$350,000 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.

LAWRENCE LIVERMORE NATIONAL LABORATORY
P. O. Box 808
Livermore, CA 94550

Metals and Ceramics - 01 -

R. M. Alire - Phone (FTS) 532-6340 or (415) 422-6340

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.

LAWRENCE LIVERMORE NATIONAL LABORATORY (continued)

192. OPTICAL MATERIALS RESEARCH

L. L. Chase, D. Milam, S. Payne, W. Siekhaus, N. Winter
Phone: (415) 422-6270

$687,000 02-2

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 photoemission of electrons and ions, time-of-flight mass spectroscopy surface chemical analysis, and optical emission from laser-excited surfaces.

LOS ALAMOS NATIONAL LABORATORY
P. O. Box 1663
Los Alamos, NM 87545

Metallurgy and Ceramics

S. S. Hecker - Phone (FTS) 843-9243 or (505) 667-9243

200. THE EFFECT OF SELF-IRRADIATION ON STABILITY OF CERAMIC NUCLEAR WASTE

F. W. Clinard Jr.
Phone: (505) 667-5102

$310,000 01-4

Alpha decay self-damage in zirconolite, perovskite, pyrochlore, and multiphase SYNROC ceramic waste. Doping with short half-life actinides and examination of natural mineral analogues. Role of starting composition and crystal structure. Evolution of the metamict state, localized and generalized atomic disorder, alpha recoil tracks. Simulation of damage by ion irradiation. Characterization of damage effects by X-ray and electron diffraction, optical and electron microscopy, EXAFS, dilatometry, calorimetry, and fractography. Changes in density (swelling), microhardness, fracture toughness, and resistance to microcracking. Effect of elevated temperature during self-damage, post-irradiation annealing and recovery.

201. MECHANICAL PROPERTIES

M. G. Stout, U. F. Kocks, P. S. Follansbee, P. L. Martin,
D. J. Srolovitz
Phone: (505) 667-6750

$750,000 01-5

Response of metals to multiaxial loading and large strains, yield surfaces, multiaxial stress-strain relationships, stress path changes. Characteristics of and mechanisms controlling the large strain deformation of aluminum, nickel, copper, brass, substructural and textural evolution with strain and strain state. Predictions of texture evolution using crystal plasticity and strain-rate sensitivity. Kinetics of plastic flow at room and elevated temperatures. Response of metals to high strain rates, Hopkinson split-pressure bar experiments, dislocation dynamics, viscous drag. Multi-axial loading, brittle-fracture responses of Al_2O_3, Si_3Ni_4, SiC and ZrO_2, statistical fracture theories for mixed-mode fracture of indention-producted surface flaws and microscopic cracks, microstructural effects on multiaxial loading brittle fracture. Dynamics of microstructural evolution, Monte Carlo computer simulations.

LOS ALAMOS NATIONAL LABORATORY (continued)

202. STRUCTURAL CERAMICS

D. S. Phillips, J. J. Petrovic
Phone: (505) 667-4481

$300,000 01-5

Reactivity of SiC and Al_2O_3 powders in selected non-aqueous media, and their consequent electrophoretic mobility. Correlation of reactivity with UHV surface chemistry and with powder microstructure. Selection of surfactants for optimal dispersion stability. Packing and drying powder compacts from these dispersions, with emphasis on critical point drying. Densification of these compacts. Microstructural evolution through packing, drying, and firing, with emphasis on correlating agglomerate structures with grain boundary microstructures in the final product.

Materials Chemistry - 03 -

S. S. Hecker - Phone (FTS) 843-9243 or (505) 667-9243

203. SURFACE SCIENCE OF CERAMICS

T. N. Taylor
Phone: (505) 667-7712

$130,000 03-2

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 wtih model single crystal experiments. Surface bonding (XPS) and subsurface diffusion (RBS) of selected dopants on SiC, especially the beta-form.

204. CONDUCTING POLYMERS AS SYNMETALS

M. Aldissi, A. R. Bishop, D. K. Campbell, C. Huang, R. Liepins
Phone: (505) 667-1326

$130,000 03-2

Investigation of synthesis-structure-prroperty 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.

LOS ALAMOS NATIONAL LABORATORY (continued)

Physics Division - 02 -

F. A. Morse - Phone (FTS) 843-6162 or (505) 667-6162

205. CONDENSED MATTER RESEARCH WITH THE LANSCE FACILITY

R. N. Silver
Phone: (505) 667-6069

$1,680,000 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, chemical structure, and chemical spectroscopy. The 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, liquids, amorphous, special environment diffractometer, constant-Q spectrometer, and, in the near future, a low-Q diffractometer and a chopper spectrometer.

206. MATERIALS UNDER EXTREME CONDITIONS

R. L. Mills, R. LeSar, D. Schiferl
Phone: (505) 667-4129

$240,000 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.

LOS ALAMOS NATIONAL LABORATORY (continued)

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

J. C. Wheatley
Phone: (505) 667-7499

$260,000 02-5

Natural or intrinsically irreversible engines: acoustic engines using liquids and gases, magnetic engines, heat pumps and prime movers, liquid propylene thermodynamic and thermophysical properties, liquid propylene heat engine: regenerators, heat exchangers, mechanicals, seals, thermal convection in dilute solutions of ^{3}He in superfluid ^{4}He near 1 K, steady and oscillatory, nonlinear dynamics, coherence and chaos, spin-polarized hydrogen isotopes: transport, thermodynamic properties, megnetosound, normal and superfluid liquid ^{3}He: ferromagnetism, susceptibility anisotropy.

OAK RIDGE NATIONAL LABORATORY
P. O. Box X
Oak Ridge, TN 37831

Metallurgy and Ceramics - 01 -

J. O. Steigler - Phone (FTS) 624-4065 or (615) 574-4065

215. THEORETICAL STUDIES OF METALS AND ALLOYS

J. S. Faulkner, W. H. Butler, G. S. Painter, G. M. Stocks, D. M. Nicholson
Phone: (615) 574-5161

$700,000 01-1

KKR-CPA method for calculating the electronic states of alloys to provide the basis for explaining experiments on alloy systems such as photoemission, positron annihilation, soft X-ray emission and adsorption, resistivity, low-temperature specific heats, etc. Use of the high-speed band theory technique OKKR to calculate total energies of metals and intermetallic compounds. Coupling results with KKR-CPA calculations to obtain insights into the thermodynamic parameters that determine the phase stability of alloy systems. Study of magnetism at finite temperatures and of ordering and transport phenomena in alloys. Use of electron-phonon interactions are calculated to explain resistivities of normal metals and super-conductors. Application of cluster and layer techniques to calculate the physical and chemical properties of surfaces interacting with their environment. Studies of metal-metalloid clusters to study grain-boundary segregation and cohesion.

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

$640,000 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 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.

OAK RIDGE NATIONAL LABORATORY (continued)

217. MICROSCOPY AND MICROANALYSIS

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

$700,000 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 $E_0 < 300$ 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 Ni_3Al, AEM of supported metal catalysts.

218. DEFORMATION AND FRACTURE OF METALS AND ALLOYS

M. H. Yoo, J. Schneibel, C. L. White, G. F. Petersen
Phone: (615) 574-5165

$625,000 01-2

Experimental and theoretical research on the role of interfaces and impurities in high-temperature deformation and fracture of austenitic steels and intermetallic compounds, nucleation, growth, and interlinkage of grain boundary cavities, trace element segregation to grain boundaries and free surfaces, grain boundary sliding, dynamic recrystallization. This task will be combined with the High-Temperature Alloy Design Task in FY 1986.

219. MECHANICAL PROPERTIES OF CERAMICS

P. F. Becher, P. Angelini, R. K. Williams
Phone: (615) 574-5157

$520,000 01-2

Experimental and theoretical studies to describe the basis for the effects of alloying and microstructure in transformation toughening especially for ceramics containing dispersed ZrO_2 and for partially stabilized ZrO_2, on subcritical crack growth. This task will be combined with the Processing Science and Mechanical Behavior of Ceramics Task in FY 1986.

OAK RIDGE NATIONAL LABORATORY (continued)

220. METASTABLE MATERIALS

D. M. Kroeger, D. S. Easton, C. G. McKamey
Phone: (615) 574-5155

$395,000 01-3

Relationships among composition, structure, and physical properties of metallic glasses, glass stability, effects of impurity additions on structure and properties of metallic glasses, preparation techniques by arc-hammer, melt-spinning and electron-beam vapor deposition, mechanical properties, low-temperature specific heat, small-angle scattering and TEM studies of defect structure, and phase separations in metallic glasses. This work will be concluded at the end of FY 1985.

221. 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

$1,570,000 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 void nucleation and growth, phase stability under irradiation, ion-irradiation studies using multiple ion beams (heavy and dual light ions), relationship between ion and neutron damage, effect of helium and other gases on nucleation and growth of voids and interstitial loops, theory of void and loop nucleation and growth, solute-defect interactions, irradiation creep, cascade diffusion theory, Fe, Al, Zr, Ni, and alloys, stainless steels, ferritic alloys, ceramics.

OAK RIDGE NATIONAL LABORATORY (continued)

222. HIGH TEMPERATURE ALLOY DESIGN

C. T. Liu, C. L. White, D. M. Kroeger, M. H. Yoo, J. H. Schneibel, R. K. Williams, J. A. Horton, W. C. Oliver, A. DasGupta
Phone: (615) 574-4459

$330,000 01-5

Design of ordered intermetallic alloys based on Ni_3Al aluminides, microalloying and grain-boundary segregation. Effect of alloy stoichiometry on structure and properties of grain boundaries, nature and effects of point defects, dislocation structure in deformed aluminides, solid solution hardening, deformation and fracture behavior at elevated temperatures, grain-boundary cavitation in creep tests, theoretical modeling of creep behavior of nickel aluminides, superplastic behavior, free-surface and grain-boundary segregation of boron, environmental effects on crack nucleation and growth, structure and properties of rapidly solidified aluminides, studies of physical properties, establish correlation between properties, microstructure, and defect structures in aluminides.

223. PROCESSING SCIENCE AND MECHANICAL BEHAVIOR OF CERAMICS

P. F. Becher, P. Angelini, A. Bleier, R. K. Williams
Phone: (615) 574-5157

$390,000 01-5

Experimental and theoretical studies of ceramic processing including role of particulate synthesis, surface chemistry and physical characteristics on dispersion behavior and agglomeration and ordering in consolidated particulates, mechanisms of sintering and microstructural evolution in single and multiphase systems (e.g., TiB_2, ZrO_2, Al_2O_3-ZrO_2), characterization and modeling of crack growth behavior of such ceramics with respect to transformation mechanisms (e.g., ZrO_2), grain boundary effects and crack tip interactions with microstructural features (e.g., second phases).

224. FUNDAMENTALS OF WELDING AND JOINING

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

$400,000 01-5

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 Technology Application Center (AWTAC) Projects.

OAK RIDGE NATIONAL LABORATORY (continued)

225. STRUCTURE AND PROPERTIES OF SURFACES AND INTERFACES

C. J. McHargue, P. S. Sklad, C. S. Yust, M. B. Lewis, R. A. McKee, P. Tortorelli
Phone: (615) 574-4344

$615,000 01-5

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

226. DIRECT PROCESSING OF NEAR NET SIZE STEEL CASTINGS TO FINAL PRODUCTS

V. K. Sikka, D. O. Hobson
Phone: (615) 574-5112

$200,000 01-5

Development of a scientific basis for the use of thermal mechanical processing for controlling the properties of steels, development of experimental facilities for simulating or for duplicating on a laboratory scale complex sequences of thermal and mechanical processing steps, processing of thin cross section materials produced by the task on Electromagnetic Continuous Casting of Steel conducted at ANL. The experimental facilities developed and maintained by this task will be operated in a user mode to enable individual steel companies to carry out alloy or processing development programs to develop steels to meet the needs of their customers. Steel industry employees will participate in most of the work.

OAK RIDGE NATIONAL LABORATORY (continued)

Solid State Division - 02 -

M. K. Wilkinson - Phone (FTS) 624-6151 or (615) 574-6151

227. INTERATOMIC INTERACTIONS IN CONDENSED SYSTEMS

R. M. Nicklow, J. R. Arthur, J. W. Cable, H. R. Child, M. Hagen, J. B. Hayter, S. Kawarazaki, W. C. Koehler, P. Kumar, H. A. Mook, R. M. Moon, O. A. Pringle, H. G. Smith, W. G. Stirling N. Wakabayshi
Phone: (615) 574-5240

$1,095,000 02-1

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 $KMgF_3$, UBe_{13}, $BaLaGa_3O_7$, and graphite intercalated with D_2SO_4, magnetic excitations in spin glasses, USb, paramagnetic Ni and Fe, Pt_3Mn, and $KMn(Ni)F_3$, phase transitions in Sn, $RbNO_3$, Ni_3Mn, $SmSn_3$, Cu(Fe), and random-field systems, nuclear spin ordering in Pr, $PrCu_2$, and VBr_2, momentum distributions in ^3He and ^4He. New research directions will include more emphasis on materials properties under extreme environments of high pressures, high temperatures or ultralow temperatures.

228. PROPERTIES OF DEFECTS, SUPERCONDUCTORS, AND HYDRIDES

J. W. Cable, R. Arons, J. R. Arthur, H. R. Child, W. C. Koehler, J. B. Hayter, H. A. Mook, R. M. Moon, Y. Morii, R. M. Nicklow, O. A. Pringle, H. G. Smith, S. Spooner, G. D. Wignall
Phone: (615) 574-5233

$770,000 02-1

Elastic, inelastic, and small-angle scattering of neutrons by superconductors, metal hydrides, and defects in single crystals, lattice dynamics of CeD_2, Fe(Cr) alloys, and KCl(CN), magnetic excitations in CeD_2 and PrD_2, phase transitions in 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.

OAK RIDGE NATIONAL LABORATORY (continued)

229. SUPPORT FOR NEUTRON USERS' PROGRAM

H. A. Mook, J. W. Cable, H. R. Child, H. R. Hagen, R. M. Moon, R. M. Nicklow, O. A. Pringle, H. G. Smith
Phone: (615) 574-5242

$495,000 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, structure and dynamics of spin glasses, random field systems, polarized-beam studies of paramagnetism, heavy fermion superconductors, amorphous magnetic materials, proton diffusion in biological systems, and collagen periodicity in bones.

230. PHYSICAL PROPERTIES OF SUPERCONDUCTORS

S. T. Sekula, Y. K. Chang, D. K. Christen, J. R. Ellis, H. R. Kerchner, D. H. Lowndes, J. R. Thompson
Phone: (615) 574-6271

$440,000 02-2

Investigations of flux-line-lattice arrays, flux motion, flux-line defect interactions, anisotropy in refractory metal alloys and compounds with A15 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.

OAK RIDGE NATIONAL LABORATORY (continued)

231. SEMICONDUCTOR PHYSICS AND PHOTOPHYSICAL PROCESSES OF SOLAR ENERGY CONVERSION

R. F. Wood, M. J. Aziz, E. Fogarassy, G. E. Jellison,
D. H. Lowndes, F. A. Mashburn, F. A. Modine, S. J. Pennycook,
R. Ruckteschler, R. D. Westbrook, S. P. Withrow
Phone: (615) 574-5781

$870,000 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.

232. FUNDAMENTAL ASPECTS OF METAL FRACTURE

S. M. Ohr, S.-J. Chang, C. G. Park
Phone: (615) 574-5509

$465,000 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.

OAK RIDGE NATIONAL LABORATORY (continued)

233. HIGH TEMPERATURE CERAMIC MATERIALS

J. B. Bates, F. A. Modine, C. Y. Allison, Y. Chen, Y. T. Chu,
N. J. Dudney, G. R. Gruzalski, E. Sonder, J. C. Wang
Phone: (615) 574-6151

$930,000 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 conductivity in AgCl-Al_2O_3 composites, techniques include optical and electron spectroscopies and electrical measurements.

234. SOLID-SOLID INTERFACES

J. B. Bates, D. M. Zehner, Y. T. Chu, J. C. Wang
Phone: (615) 574-6151

$145,000 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.

OAK RIDGE NATIONAL LABORATORY (continued)

235. PREPARATION AND CHARACTERIZATION OF RESEARCH MATERIALS

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

$690,000 02-2

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 reduction float zone growth of transition-metal carbide single crystals, growth of perovskite-structure oxides (e.g., $KTaO_3$, $CaTiO_3$, $KTa_{1-x}Nb_xO_3$), float zone and tri-arc growth of A15 compounds (i.e., V_3Si, Ti_3Pt, 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.

236. SMALL-ANGLE X-RAY SCATTERING

W. C. Koehler, J. S. Lin, S. Spooner
Phone: (615) 574-5232

$160,000 02-2

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 transformatiaon. Facilities are available to users through National Center for Small-Angle Scattering Research (NCSASR).

OAK RIDGE NATIONAL LABORATORY (continued)

237. THEORY OF CONDENSED MATTER

J. F. Cooke, J. H. Barrett, H. L. Davis, W. Ekardt, L. J. Gray, T. Kaplan, S. H. Liu, G. D. Mahan, M. E. Mostoller, O. S. Oen, A. K. Rajagopal, M. Rasolt, M. T. Robinson, K. Shung, K. R. Subbaswamy, J. C. Wang, R. F. Wood
Phone: (615) 574-5787

$1,230,000 02-3

Theory of laser annealing, laser-induced diffusion, and nonequilibrium solidification in semiconductors, lattice vibrations in metals and alloys, lattice dynamics and potential energy calculations of ionic crystals, computer simulation of radiation damage and sputtering, reflection of light atoms from surfaces, surface studies with backscattered ions, development of LEED theory and interpretation of LEED data, surface vibrations and relaxation, theory of angular effects in photoemission, electronic structure of metal surfaces, magnetism in transition metals and local moment systems, electronic properties of mixed-valent systems, critical phenomena and phase transitions. New directions include: quantum Hall effect, neutron scattering at high energies, development and application of SPLEED theory, diffusion and elastic vibrations of fractal systems.

238. X-RAY DIFFRACTION AND ELECTRON MICROSCOPY

B. C. Larson, J. Narayan, S. D. Berger, J. D. Budai, J. D. Lewis, T. S. Noggle, S. M. Ohr, C. G. Park, S. Pennycook, J. Z. Tischler
Phone: (615) 574-5506/5508

$825,000 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 assocated 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.

OAK RIDGE NATIONAL LABORATORY (continued)

239. SYNTHESIS AND PROPERTIES OF ISOTOPIC SOLIDS

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

$430,000 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.

240. ESTABLISHMENT AND RESEARCH USE OF A NATIONAL LOW-TEMPERATURE IRRADIATION FACILITY

R. R. Coltman Jr., C. E. Klabunde
Phone: (615) 574-6263

$635,000 02-4

Construct, test, and operate for users a National Low-Temperature Neutron Irradiation Facility (NLTNIF) 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.

OAK RIDGE NATIONAL LABORATORY (continued)

241. SURFACE PHYSICS AND CATALYSIS

L. H. Jenkins, H. L. Davis, R. A. DiDio, J. R. Gruzalski, J. R. Noonan, J. F. Wendelken, C. W. White, D. M. Zehner
Phone: (615) 574-7031

$950,000 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.

242. SURFACE MODIFICATION AND CHARACTERIZATION FACILITY AND COLLABORATIVE RESEARCH CENTER

B. R. Appleton, O. E. Schow III, T. P. Sjoreen, C. W. White
Phone: (615) 574-6283

$935,000 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.

OAK RIDGE NATIONAL LABORATORY (continued)

243. ION BEAM ANALYSIS AND ION IMPLANTATION

B. R. Appleton, C. W. White, M. J. Aziz, J. H. Barrett, T. B. Cook, R. J. Culbertson, G. C. Farlow, N. Herbots, E. Kelly, C. J. McHargue, D. B. Poker, O. E. Schow, J. M. Williams, S. Withrow
Phone: (615) 574-6283

$1,030,000 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.

244. RESEARCH AND DEVELOPMENT - ISOTOPE RESEARCH MATERIALS PREPARATION

H. L. Adair, W. S. Aaron, M. Petek, T. C. Quinby, D. W. Ramey
Phone: (615) 574-5900

$355,000 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, reactive and 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, micorgravimetric determinations, thermal conductivity determination, in situ film thickness monitoring, and sophisticated radiation counting methods.

OAK RIDGE NATIONAL LABORATORY (continued)

Materials Chemistry - 03 -

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

245. CHEMISTRY OF ADVANCED INORGANIC MATERIALS

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

$1,218,000 03-1

Application of ion implantation and related nonequilibrium processing techniques 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 Cl_2 and O_2 evolution, development of in-situ photo-acoustic spectroscopy for determining the nature and thickness of thin oxide layers on metals. SiS-based methodology for the synthesis of high-purity ceramics (Si_3N_4, SiC, etc.) from relatively impure silicon, synthesis, characterization, and pyrolysis of groups IV-A, V-A, and VI-A transition metal organometallic compounds for the preparation of ceramic powders, films, and fibers, metathetical and solvolytic reactions in oxygen-free nonaqueous media (e.g. liquid ammonia, molten cyanides) for the synthesis of nonoxide ceramic precursors and compounds, application of metal atom reactor to the synthesis of ceramic materials.

246. STRUCTURE AND DYNAMICS OF ADVANCED POLYMERIC MATERIALS

A. H. Narten, B. K. Annis, G(eorge) M. Brown, W. R. Busing, E. Johnson, D. W. Noid, W. E. Thiessen
Phone: (FTS) 624-4974 or (615) 574-4974

$1,057,000 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.

OAK RIDGE NATIONAL LABORATORY (continued)

247. THERMODYNAMICS AND SENSITIVITY ANALYSES INVOLVING ENERGY-RELATED MATERIALS

T. B. Lindemer, C. A. Culpepper
Phone: FTS 624-6850 or (615) 574-6850

$371,000 03-2

Determination and modeling of phase equilibria and other thermochemical data important to energy-producing systems. Emphasis on the measurement and application of such data for the actinide oxides used as nuclear fuels, but the methodology applicable to any oxide solid solution. Current studies involve relevant subsystems in the system of elements U, Pu, O, and specific fission products, particularly lanthanides. Experimental data obtained under conditions generally not previously investigated. Adaptations of chemical- mathematical models from the literature used to represent the chemical thermodynamic interrelationship of temperature, oxygen chemical potential, and nonstiochiometry reported in the literature. These efforts provide a heretofore unavailable, generalized chemical thermodynamic description of the actinide-lanthanide dioxide solutions.

248. CHEMICAL ENGINEERING RESEARCH

C. H. Byers, D. F. Williams, M. T. Harris
Phone: (FTS) 624-4653 or (615) 574-4653

$302,000 03-2

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.

OAK RIDGE ASSOCIATED UNIVERSITIES
Oak Ridge, TN 37831

Metallurgy and Ceramics - 01 -

Richard Wiesehuegel - Phone (FTS) 626-3383 or (615) 576-3383

255. OAK RIDGE SYNCHROTRON ORGANIZATION FOR ADVANCED RESEARCH

T. A. Habenschuss, C. J. Sparks, R. DeAngelis, S. Moss, R. Young
Phone: (615) 574-6996

$100,000 01-1

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 will supply 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 rearrangements.

256. SHARED RESEARCH EQUIPMENT PROGRAM (SHARE)

E. A. Kenik, J. L. Lehman
Phone: (615) 574-5066

$97,923 01-1

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.

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

Metallurgy and Ceramics - 01 -

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

260. HIGH-TEMPERATURE CORROSION AND ELECTROCHEMICAL INTERACTIONS IN CERAMICS

J. L. Bates, M. J. Danielson
Phone: (509) 375-2579

$310,000 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 $MgAl_2O_4$, Al_2O_3, MgO, and $Y_3Al_5O_{12}$ with Ca-Al-silicate containing Mg and Fe in oxidizing, reducing, and sulphur-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 couples 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,
M. T. Thomas
Phone: (509) 376-4276

$420,000 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. 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_2O, and H_2O+Cl) on adsorption processes studied with an in situ Auger electron spectroscopy straining stage.

PACIFIC NORTHWEST LABORATORY (continued)

262. LEACHING OF GLASS AND CERAMICS

G. L. McVay, L. R. Pederson, D. S. Goldman, B. P. McGrail, C. J. Hostetler
Phone: (509) 375-3762

$350,000 01-3

Mechanistic studies of the interactions of silicate glasses and crystalline ceramics with water, 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.

263. RADIATION EFFECTS IN METALS AND CERAMICS

E. P. Simonen, J. L. Brimhall, G. J. Exarhos, E. R. Bradley, L. A. Charlot, C. H. Henager Jr., W. J. Weber
Phone: (509) 376-3124

$560,000 01-4

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.

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, J. W. Griffin
Phone: (509) 375-6907

$230,000 02-2

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, stochiometry, phase structure, strain, and stress. Optical and material characterization techniques Raman spectroscopy, X-ray diffraction, laser interferometry, total integrated and angular scattering, and resonant cavity reflectometry.

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

Metallurgy and Ceramics - 01 -

P. S. Peercy - Phone (FTS) 844-4309 or (505) 844-4309

275. 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, L. E. Pope, R. B. Diegle, N. R. Sorensen
Phone: (505) 844-7681

$890,000 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, channeling in superlattices, defects in semiconductors, rapid-solidification proceses 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.

R. J. Eagan - Phone (FTS) 844-4069 or (505) 844-4069

276. PHYSICS AND CHEMISTRY OF CERAMICS

T. A. Michalske, A. Hurd, D. Haaland, B. C. Bunker, K. D. Keefer, D. W. Schaefer, C. J. Brinker
Phone: (505) 846-3551

$555,000 01-2

Multidisciplinary studies to relate molecular structure of ceramics to physical properties. Develop models for environment/strained solid interactions. Photon Stimulated Desorption (PSD) of in situ fracture surfaces to determine chemical compounds resulting from stress corrosion fracture, molecular orbital (MO) calculations to predict reactivity of mechanically strained crack tip bonds, model systems to study strain-enhanced chemistry, FTIR studies of adsorbate reactions to relate strain enhanced chemistry and stress corrosion fracture. Characterize sol-to-gel and gel-to-glass transitions in silica system using SAXS, HPLC, NMR, and light scattering to determine structures of pre-gel phase, random colloidal aggregates, and gel-to-glass conversion, model structure of porous materials using concepts of fractal geometry to predict structure from solution chemistry, and model sintering and absorption characteristics of random porous materials.

SANDIA NATIONAL LABORATORIES - ALBUQUERQUE (continued)

277. STRAINED-LAYER SUPERLATTICE MATERIALS SCIENCE

R. M. Biefeld, L. R. Dawson, I. J. Fritz, P. L. Gourley, D. R. Myers, G. C. Osbourn
Phone: (505) 844-1556

$550,000 01-2

Studies of strained-layer superlattices (SLS's), a new class of semiconductor materials with unique and tailorable electronic and structural properties are expected to have a broad range of device applications. Research emphasizes: electronic energy levels and the effects of Brillouin zone folding on optical transition strengths in SLSs, transport properties and quantum oscillations in SLS structures tailored for large mobilities, conditions for growth and doping of new SLS structures, stability of SLS's subjected to high temperature aging, ion implantation damage and annealing, thermal cycling, and hydrostatic pressure.

Solid State Physics - 02 -

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

278. SURFACE PHYSICS RESEARCH AND STIMULATED DESORPTION

J. E. Houston, D. R. Jennison, G. L. Kellogg, R. R. Rye, R. Stulen, A. R. Burns
Phone: (505) 844-6653

$700,000 02-2

Developing fundamental understanding at local atomic level of physics underlying modification and control of surfaces by studies of electronic and structural properties. Near term emphasis on oxidation, adhesion, promotion and poisoning of catalytic activity, and radiation induced damage and chemistry. Strong features are the ability (1) to bring to bear a number of techniques which probe the properties of modified surfaces at the local atomic level, (2) to couple with theoretical support, and (3) to have direct relationships with applied programs in a multidisciplinary approach which ensures technological impact. Program encompasses experimental and theoretical efforts in Auger lineshape analysis, LEELS, UPS, the Pulsed-Laser Atom Probe, and stimulated desorption which includes a new laser-based, state-selective neutral desorption technique.

SANDIA NATIONAL LABORATORIES - ALBUQUERQUE (continued)

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

279. ORGANIC CONDUCTORS AND SUPERCONDUCTORS

L. J. Azevedo, D. S. Ginley, J. F. Kwak, P. F. Nigrey, J. E. Schirber
Phone: (505) 846-2529

$300,000 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.

Materials Chemistry - 03 -

J. B. Gerardo - Phone (FTS) 844-3871 or (505) 844-3871

280. 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

$440,000 03-3

Studies of important vapor-phase reactions and nucleation processes during CVD deposition under conditions used to fabricate photovolataic 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.

SANDIA NATIONAL LABORATORIES
Livermore, CA 94550

Metallurgy and Ceramics - 01 -

D. L. Hartley - Phone (FTS) 532-2747 or (415) 422-2747

290. SURFACE LAYER EVOLUTION IN DEPOSIT-FORMING FLOWS

M. Lapp, A. S. Nagelberg, R. J. Anderson, K. F. McCarty
Phone: (415) 422-2435

$300,000 01-1

Studies of the initial stages of deposition phenomena underlying fouling, slagging, and corrosion for materials exposed to combustion environments. Utilize in situ, nonintrusive optical diagnostics for multiphase, multicomponent systems. Primary emphasis on Raman spectroscopy applied to substrates in well-controlled laboratory combustion flow reactors. Include numerical computations of impinging flow from boundary layer and realistic physical chemistry to determine broad range of gas-surface interactions that affect surface conditions.

291. GASES IN METALS/COMPUTATIONAL METALLURGY

M. I. Baskes, G. J. Thomas, M. S. Daw, S. M. Foiles, W. G. Wolfer, S. Robinson, S. Goods, C. F. Melius, J. S. Binkley
Phone: (FTS) 532-3226 or (415) 422-3226

$460,000 01-2

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_3Al, both in the bulk and at interfaces including the effects of adsorbates and alloying additions.

SANDIA NATIONAL LABORATORIES - LIVERMORE (continued)

292. THIN SURFACE LAYER REACTIONS

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

$239,000 02-2

Develop and evaluate advanced diagnostic techniques for combustion-related materials research to produce in situ, real time, nonperturbing data. Focus upon initial changes in surface conditions when exposed to combustion environment in studies of species and reactions at interfaces typical of combustion systems. Emphasis on probing surface and near-surface layers with Raman scattering, including capability to use micro-Raman spectroscopy with a hot stage. New thrust into development of surface monolayer probes based on nonlinear optical spectroscopic techniques.

SOLAR ENERGY RESEARCH INSTITUTE
1617 Cole Boulevard
Golden, CO 80401

Materials Research Branch - 01 -

G. E. Gross - Phone (FTS) 327-1228 or (303) 231-1228

295. POLYMER/THIN-FILM PHOTO AND CATALYTIC DEGRADATION RESEARCH

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

$210,000 01-1

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 polymethylethracrylate, polyacarbonate, and polypropylene in contact with copper oxide, silver chloride, or copper, silver, and 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.

Solid State Research Branch - 02 -

S. Deb - Phone (FTS) 327-1105 or (303) 231-1105

296. SEMICONDUCTOR THEORY

A. Zunger
Phone: (303) 231-1172

$140,000 02-3

Theoretical studies of electronic properties of new ternary semiconductors and binary, ternary ordered and disordered alloy systems: predict chemical trends and properties of new materials of potential photovoltaic interest, prediction of structural parameters and relative stabilities of these systems. Systems: ordered and disordered A_xB_{1-x} and $A_xIIIB_{1-x}IIICV$ tetrahedrally bonded (e.g. SiGe, $Ga_nIn_mP_{n+m}$) alloys, Nowotny-Juza ($A^IB^{II}CV$) compounds (e.g., LiZnP) and antifluorite compounds (e.g., Mg_2Si), ternary pnictides ($ZnBC_2$ for B=Si, Ge,Sn and C=As,P). Theoretical methods: total energy non-local pseudo-potential method, all-electron Mixed Basis Potential Variation band structure method. Study of deep defects in semiconductors: chemical trends for 3rd impurity levels in different hosts (including alloys), predict hitherto unobserved impurity levels and excited states and the lattice distortions induced in the host, clarify their likely impact on device characteristics. Theoretical techniques: Quasi-Band Crystal Field Green's function method, modified multiplet-corrected formalism with self-interaction corrections.

STANFORD SYNCHROTRON RADIATION LABORATORY
Stanford University
P. O. Box 4349, Bin 69
Stanford, CA 94305

Solid State Physics - 02 -

A. I. Bienenstock - Phone (FTS) 461-9300 or (415) 854-3300, X 3153

298. RESEARCH AND DEVELOPMENT OF SYNCHROTRON RADIATION FACILITIES

A. I. Bienenstock, G. S. Brown, H. Winick
Phone: (415) 854-3300 Ext. 3153

$1,140,000 02-2

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

Contract and Grant Research

(Primarily Universities)

The information in this Section was prepared by the DOE project monitors of the Division of Materials Sciences. There is considerable turnover in the Contract and Grant Research program and some of the projects will not be continued beyond the current contract period. (The Division is in the process of changing its mode of funding basic research from contracts to grants. No distinction is made between these modes in this Section.)

ARIZONA STATE UNIVERSITY
Tempe, AZ 85281

301. IMAGING OF SURFACES AND DEFECTS OF CRYSTALS

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

$104,067 02-2

Application of advanced electron optical techniques to the study of the structure of crystal surfaces and their surface reactions. Micro-diffraction, surface imaging and electron energy loss spectroscopy combined with high resolution imaging in studies of the structure and reactions of the surfaces of metal and oxide crystals. The influence of crystal defects and the effects of ionizing radiation on surface reactions.

UNIVERSITY OF ARIZONA
Tucson, AZ 85721

302. ARTIFICIALLY LAYERED SUPERCONDUCTORS

C. M. Falco
Dept. of Physics
Phone: (602) 626-1866

$80,000 02-2

Investigation of the structure of artificial metallic multilayer systems, their electronic and superconducting properties including their weak link characteristics. Produce superlattices with higher perfection than theretofore, and understand what are the important preparation parameters. Fabricate layered materials with a three-gun magnetron sputtering system and use X-ray diffraction, resistance, Rutherford backscattering, TEM, electron tunneling to characterize the samples. Emphasis on the superconducting properties of the superlattice systems to develop weak links and microbridges with increased range of operating conditions.

BATTELLE COLUMBUS LABORATORIES
Columbus, OH 43201

303. MULTIAXIAL STRESS RESPONSE OF CERAMICS

A. R. Rosenfield
Phone: (614) 424-6424
D. K. Shetty
Phone: (614) 424-6424
W. Duckworth
Phone: (614) 424-6424

$165,000 01-5

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: Al_2O_3, Si_3N_4, glass-ceramics, and partially stabilized ZrO_2.

BOEING AEROSPACE COMPANY
Seattle, WA 98124

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

$84,990 01-1

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.

BOSTON UNIVERSITY
Boston, MA 02215

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.

BRANDEIS UNIVERSITY
415 South Street
Waltham, MA 02254

306. TWO-DIMENSIONAL COLLOIDAL SYSTEMS

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

$48,287 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 10μm) permits both exploration of reciprocal space by coherent light scattering and direct real space observations by optical microscopy.

BRANDEIS UNIVERSITY (continued)

307. SYNTHESIS AND PROPERTIES OF NOVEL, ELECTROACTIVE ORGANOMETALLIC POLYMERS

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

$77,100 03-1

Synthesis of a number of organometallic polymers based on transition metal complexation of rigidly held aromatic five and six membered rings. The aromatic rings will be held in a framework such that electron or hole conduction should occur through overlap of the -orbitals on contiguous facing aromatic rings. The C_6-based polymers will be derived from paracyclophenes and the C_5 polymers from cyclopentadienylnaphthalene.

BRIGHAM YOUNG UNIVERSITY
Provo, UT 84601

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

B. L. Adams
Dept. of Materials Science and Engineering
Phone: (904) 392-6617

$53,000 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.

BROWN UNIVERSITY
Providence, RI 02912

309. A COMBINED MACROSCOPIC AND MICROSCOPIC APPROACH TO THE FRACTURE OF METALS

R. J. Asaro
Div. of Engineering
Phone: (401) 863-2868
J. Gurland
Div. of Engineering
Phone: (401) 863-2868
A. Needleman
Div. of Engineering
Phone: (401) 863-2868
C. F. Shih
Div. of Engineering
Phone: (401) 863-2868

$225,000 01-2

Theoretical and experimental studies of fracture in metals, principally steels, combined theoretical and experimental studies of crack tip deformation and micro-fracture processes at crack tips, finite element modelling of crack tip behavior including studies of yield surface vertices on crack tip fields, correlations of microstructure and fracture toughness of dual phase and quenched and tempered martensitic steels, time dependent crack tip deformation and finite element modelling of creep deformation at crack tips, applications to engineering fracture mechanics, hydrogen assisted fractures in steels.

310. CONCURRENT USE OF STRESS PULSES AND ULTRASONIC WAVES TO STUDY EFFECTS OF RAPID STRAIN ON THE INTERNAL STRUCTURE OF SOLIDS

C. Elbaum
Div. of Applied Mathematics
Phone: (401) 863-2186
A. Hikata
Div. of Applied Mathematics
Phone: (401) 863-2187

$105,500 01-2

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.

BROWN UNIVERSITY (continued)

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

$42,830 (6 Months) 01-2

Experimental study of the influence of compression cycles on the growth of cracks in steels under constant and variable amplitude fatigue loading conditions, modelling of the micromechanisms of cyclic crack advance under continuous and periodic compression loading. Analyses of the role of crack closure as a function of microstructure, load ratio, and environment under far-field cyclic compression.

312. NOVEL DYNAMIC INVESTIGATIONS OF EXCITONS AND THEIR STRUCTURE IN SEMICONDUCTORS

A. V. Nurmikko
Div. of Engineering
Phone: (401) 863-2869

$79,033 02-2

Characteristics and energetics of excitons in selected semi-conductors studied from a dynamical point of view. Subnanosecond laser sources and transient spectroscopy used to obtain information about energy relaxation and localization and the effect of screening of an interacting excitonic gas. Materials include Cu_2O, TlBr and (Zn, Mn)Te mixed crystals.

CALIFORNIA INSTITUTE OF TECHNOLOGY
Pasadena, CA 91125

313. STUDIES OF ALLOY STRUCTURE AND PROPERTIES

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

$297,000 01-1

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 not prepared by rapid quenching. Atomic structure studies include use of EXAFS, XANES, SAXS, SANS, X-ray Raman scattering, Mossbauer spectroscopy, and NMR. Electronic structure is probed by measuring specific heats, transport properties and superconductivity.

314. MELTING IN ADSORBED FILMS

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

$102,199 02-2

Experimental study of the relation between dimensionality and phase transitions, especially melting, in multilayer adsorbed films. Comprehensive thermodynamic measurements together with pulsed nuclear magnetic resonance is used to study the interaction of melting with wetting, roughening and other surface related phenomena. A prototypical study: multilayer methane adsorbed on graphite foam.

UNIVERSITY OF CALIFORNIA/DAVIS
Davis, CA 95616

315. RADIATION DAMAGE AND DURABILITY OF NUCLEAR WASTE STORAGE MATERIALS

D. G. Howitt
Dept. of Mechanical Engineering
Phone: (916) 752-1164

$94,000 01-1

Evaluation of fundamental processes of radiation damage in silicate based glasses and the leaching behavior of multicomponent glasses and ceramics. Concerns include the chemical role of helium in the radiation damage process, the size of damage volumes involved in the crystalline to amorphous transformation, and the radiation damage processes that contribute to the radiolytic decomposition of cements.

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.

UNIVERSITY OF CALIFORNIA/DAVIS (continued)

317. AN INVESTIGATION OF THE ROLE OF SINTERING IN GAS-SOLID INTERACTIONS

Z. A. Munir
Dept. of Mechanical Engineering
Phone: (916) 752-0559

$70,000 01-3

Investigation of the role of sintering in the kinetics of gas-solid interactions in powder compacts, including both oxidation-reduction and dissociation reactions of the oxides and sulfides of iron. Study of state of division of oxides resulting from the decomposition of hydroxides and carbonates as a function of gas pressure, temperature, and impurities. Evaluation of changes of oxide particle shape and size as a function of sintering parameters. Morphological changes such as surface area, pore size, and overall porosity are measured and related to changes in the reversibility and rates of reactions. The role of sintering is elucidated by thermogravimetric, microscopy, and surface area measurement techniques. Effect of precombustion (diffusional) processes on the combustion synthesis of ceramic and metallic phases.

UNIVERSITY OF CALIFORNIA/IRVINE
Irvine, CA 92717

318. RAMAN SPECTROSCOPY OF MOLECULAR ADSORBATES

J. C. Hemminger
Dept. of Chemistry
Phone: (714) 833-6020
S. Ushioda
Dept. of Physics
Phone: (714) 833-6619

$157,500 02-2

Combine Raman spectroscopy and modern surface science technology to study binding and chemistry of adsorbates on well characterized surfaces. Study mechanism of "giant" enhanced Raman scattering. Correlate enhancement with surface roughness on stepped and kinked surface of Ag. Also correlate enhancement with electronic energy levels of metal-adsorbate system as determined by electron energy loss spectroscopy. Apply Raman spectroscopy to study of corrosion by H_2S and O_2.

UNIVERSITY OF CALIFORNIA/IRVINE

319. SURFACE EXCITATIONS AND THEIR INTERACTION WITH LOW ENERGY ELECTRONS

D. L. Mills
Dept. of Physics
Phone: (714) 833-5148

$113,000 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 with Professor Tong at the University of Wisconsin.

UNIVERSITY OF CALIFORNIA/SAN DIEGO
La Jolla, CA 92037

320. INVESTIGATION OF THE INTERACTION BETWEEN SUPERCONDUCTIVITY AND MAGNETISM AND OSCILLATORY CHEMICAL REACTIONS OVER METAL SURFACES

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

$310,000 02-2

Studies of superconductivity, magnetism and their mutual interaction in ternary and mixed ternary rare earth and uranium compounds with emphasis on "heavy Fermion" systems. Materials include ternary transition metal borides, germanides, silicides and phosphides, and ternary molybdenum chalcogenides (Chevrel phases). Effects associated with competing superconducting and magnetic interactions characterized and used to test relevant theories. Some investigations at high pressures and in high magnetic fields. Oscillatory chemical reactions, catalyzed by transition metals, studied using flow reactors and gravimetric microbalance techniques. Transition metal catalysts characterized with ultra-high vacuum LEED/Auger spectroscopy.

UNIVERSITY OF CALIFORNIA/SAN DIEGO

321. 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.

322. RESEARCH ON THE THERMOPHYSICAL PROPERTIES OF MATERIALS

J. C. Wheatley
Dept. of Physics
Phone: (505) 667-7499

$146,184 02-5

Fundamental investigations in thermal physics: Quantitative studies of intrinsically irreversible acoustic engines and other natural engines working by the same principles. Investigations of nonlinear dynamics and chaotic behavior using superfluid helium solutions as the medium. Magnetic and flow properties of He-3 at low temperatures, especially the nucleation of the superfluid B phase. Studies of homogeneous phase separation in liquid helium solutions.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA
Santa Barbara, CA 93106

323. 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

$123,000 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 of 50 to 2000 micrometers. Research on the nonlinear phenomena of phonons, and other excitations and utilizing two-phonon spectroscopy after development of techniques and facilities.

324. RESEARCH ON THE THEORY OF PATTERN FORMATION IN SYSTEMS FAR FROM EQUILIBRIUM

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

$110,644 02-3

Theoretical studies of pattern-forming processes primarily of importance to the solidification of metallurgical materials and other technological materials. Specific studies of boundary-layer model of dendritic solidification, theory of pattern selection in directional solidification of alloys, precipitation kinetics and statistical theory of the kinetics of phase separation. Further studies of phenomena in biological materials, and new theoretical techniques.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA (continued)

325. NUMERICAL SIMULATION OF QUANTUM MANY-BODY SYSTEMS

D. J. Scalapino
Physics Dept.
Phone: (805) 961-2871
J. R. Schrieffer
Physics Dept.
Phone: (805) 961-3061
R. L. Sugar
Physics Dept.
Phone: (805) 961-4078

$98,000 02-3

Development of stochastic numerical techniques for simulating many-body systems where the particles obey Fermi statistics. One-dimensional systems with various electron-phonon interactions investigated to further the fundamental understanding of conducting polymers, spin glasses and pseudo random spin systems such as $CeNiF_3$. 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.

326. SURFACE CHEMISTRY OF ELECTRO CATALYSIS

A. Hubbard
Dept. of Chemistry
Phone: (805) 961-3905

$80,000 03-3

Determination of the structure, composition and electrochemical reactivity of electrocatalyst surfaces after various stages of pretreatment and use in solutions of hydrocarbons. Comparison of the adsorption strengths of various functional groups on various metals, determination of the orientation and mode of attachment of relevant adsorbates, observation of reactivity as a function of mode of attachment and other aspects of surface state, and clarification of the role of surface structure in reactivity.

CARNEGIE MELLON UNIVERSITY
Pittsburgh, PA 15213

327. THE EFFECT OF STRESS ON PRECIPITATE MORPHOLOGY

W. Johnson
Dept. of Metallurgical Engineering and Materials Science
Phone: (412) 578-8785
D. E. Laughlin
Dept. of Metallurgical Engineering and Materials Science
Phone: (412) 578-2706

$62,067 (7 Months) 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. Alloys that may be studied: Ni-Al, Al-Li, Cu-Co. Experimental techniques include electron microscopy, X-ray diffraction.

328. THE ROLE OF PASSIVE SURFACE FILMS ON CORROSION FATIGUE CRACK PROPAGATION

I. M. Bernstein
Dept. of Metallurgical Engineering and Materials Science
Phone: (412) 578-2700
A. W. Thompson
Dept. of Metallurgical Engineering and Materials Science
Phone: (412) 578-2700
G. W. Warren
Dept. of Metallurgical Engineering and Materials Science
Phone: (412) 578-2700

$65,767 (7 Months) 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

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

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

$163,800 01-2

Ostwald ripening in ZrO_2 toughened Al_2O_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 will be 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.

UNIVERSITY OF CHICAGO
5801 S. Ellis Avenue
Chicago, IL 60639

330. 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

$40,000 (3 Months) 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.

CLARK COLLEGE
Atlanta, GA 30314

331. INVESTIGATIONS OF CHARGE TRANSPORT IN THE THERMOELECTRET STATE OF SOME GLASSES AND CERAMICS

O. P. Puri
Dept. of Natural Sciences and Mathematics
Phone: (404) 681-3080 X200

$78,888 01-3

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 $CaTiO_3$, $SrTiO_3$, $BaO_4.TiO_2$, $BiTiO_3$, $(SrBi)TiO_3$, chalcogenide glasses and elemental Se. X-ray diffraction. Thermally stimulated discharge current analysis.

COLORADO SCHOOL OF MINES
Golden, CO 80401

332. MICROSTRUCTURE AND PROPERTIES OF FERROUS ALLOY WELDMENTS

D. L. Olson
Dept. of Metallurgical Engineering
Phone: (303) 273-3787
D. K. Matlock
Dept. of Metallurgical Engineering
Phone: (303) 273-3775

$154,303 01-5

Role of Al, Cr, C and N additions on the phase stability and transformation in single pass and multiple pass Fe-Mn-Ni weld metal. Gleeble testing of Fe-Mn-Ni-Al alloys. Determination of martensite start temperature for high alloy ferrous (cryogenic) weld metal. New analytical expressions (based on fundamental concepts) for predicting weld metal microstructure and properties. Impression creep testing and modeling of heterogeneous materials (weldments). Creep behavior in heterogeneous material. High temperature mechanical degradation of ferritic-austentic dissimilar metal weldments.

UNIVERSITY OF COLORADO
Boulder, CO 80309

333. LIGHT SCATTERING STUDIES OF LOWER DIMENSIONAL COLLOIDAL PARTICLE AND CRITICAL FLUID SYSTEMS

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

$115,000 02-2

Quasi-elastic light scattering microscopy, and various other optical techniques used to study colloidal particle suspension films, monolayers, and bilipid membranes. Examination of melting/crystallization of colloidal microsphere films, experiment and computer simulations of the collapse of the particle distribution following the sudden quenching of electrostatic interparticle forces in colloidal particle monolayers on water, studies of fractal scale invariance in particle aggregates formed during coagulation, response of monolayer crystals to equivalent ultra high pressures, light scattering and reflectance studies of bilipid membranes with and without embedded microparticles and measurements of critical diffusion rates in thin films of binary liquid mixtures.

COLUMBIA UNIVERSITY
New York, NY 10027

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

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

$102,591 01-3

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 $H \leftrightarrow D$ 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.

UNIVERSITY OF CONNECTICUT
Storrs, CT 06268

335. THE FATIGUE BEHAVIOR OF FERRITIC STEELS AT ELEVATED TEMPERATURES

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

$61,107 01-2

Creep-fatigue-environmental behavior of ferritic steels (9-and 12Cr) related to strength, microstructure, oxidation resistance, fracture mechanics parameters. Influence of hold times and frequency in air and in vacuum. Determination of dominant failure mode, i.e., creep or fatigue. Modeling of the fatigue crack growth process based on range of crack opening displacement and crack closure mechanisms. Effect of temperature and mean stress on closure. Short crack growth. Fatigue crack growth in weldments. Creep crack growth.

336. ELECTRODE STUDIES IN MOLTEN SALTS

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

$11,143 01-3

Deterioration of refractory oxide films on Ni and Fe in sulfide-bearing molten salts. Field and anion effects, 'electrochemical' dissolution of oxides. Film thinning, pore formation, and structure change evaluation by impedance techniques. Formation of anodic chromium sulfides in molten sulfide salts. Current-potential characteristics of anodic sulfide films.

337. 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

$81,214 02-2

The optical properties of rare-earth-doped crystals and glasses which involve the near-ultraviolet 4f-5d transitions of the dopant ions investigated using transient and steady-state optical spectroscopy. Optical properties determined: multiphoton absorption, energy transfer, population dynamics, photo-ionization, phase conjugate wave generation, and excited-state absorption and gain.

CORNELL UNIVERSITY
Ithaca, NY 14853

338. INFLUENCE OF GRAIN BOUNDARIES ON THE ELECTRICAL PROPERTIES OF POLYCRYSTALLINE SILICON FILMS

D. G. Ast
Dept. of Materials Science and Engineering
Phone: (607) 256-4140

$60,000 (9 Months) 01-1

Characterization of the structure (high resolution TEM, electron diffraction) and electrical properties (EBIC, LIBIC, I-V, DLTS) of diffusion bonded ("welded") and as grown grain boundaries, relationship between boundary structure (esp. symmetry) and electrical activity, CSL theory, broken bond models, interactions between twins and dislocations during growth and cooling of ribbon crystals, influence of carbon (present at solubility limit in all graphite crucible grown Si) on Si self interstitial mobility, electrical activity, carbon precipitation based gettering cycles of chemical impurities.

339. THE MIGRATION OF GRAIN BOUNDARIES IN CERAMICS WITH PARTICULAR REFERENCE TO THE SINTERING PROCESS

C. B. Carter
Dept. of Materials Science and Engineering
Phone: (607) 256-4797

$202,500 01-1

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 Al_2O_3, MgO, NiO, Mg-Al spinel, Si, Ge, Si_3N_4 and 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.

CORNELL UNIVERSITY (continued)

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

S. L. Sass
Dept. of Materials Science and Engineering
Phone: (607) 256-5239
N.W. Ashcroft
Dept. of Physics
Phone: (607) 256-3309

$241,653 (10 Months) 01-1

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_3Al, 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.

341. AN INVESTIGATION OF MECHANICAL BEHAVIOUR OF POLYCRYSTALLINE SOLIDS

C-Y. Li
Dept. of Materials Science and Engineering
Phone: (607) 256-4349

$195,000 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.

CORNELL UNIVERSITY (continued)

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

S. L. Phoenix
Sibley School of Mechanical and Aerospace Engineering
Phone: (607) 256-3462

$115,000 01-2

Theoretical modelling and experimentation for the strength and creep-rupture lifetime of unidirectional composites. Statistical/micromechanical models wherein fibers fail due to randomly distributed flaws, local stress redistribution among contiguous fibers halts fracture propagation. Time dependence through viscoelasticity in the matrix leading to local creep and stochastic decay in fiber strength from thermally induced flaw growth. Calculation of short-term strength and long-term lifetime probability distributions using direct, recursive and asymptotic techniques. Creep-rupture experiments on "microcomposites" of about 20 parallel fibers impregnated with matrices varying widely in creep properties. Fibers are Kevlar 49 (aramid), S-glass and carbon. Matrices are epoxy, polyester, polyethylene and nylon 6. Special equipment constructed for fabricating and testing such composites.

343. HIGH TEMPERATURE MECHANICAL BEHAVIOR OF SILICON NITRIDE

R. Raj
Dept. of Materials Science and Engineering
Phone: (607) 256-4040

$108,000 01-2

Elucidation of the mechanisms of densification and flaw generation during high-temperature processing of powder compacts with inhomogeneous microstructures. Influence of agglomerates, non-uniform packing and second phase constituents on the densification process. Fundamental investigation of diffusion bonding of two ceramic surfaces with the aid of a liquid phase. Free sintering, hot-pressing, and sintering under superimposed hydrostatic pressure experiments on Al_2O_3 (model material for dry processing) and Si_3N_4 (with a liquid phase additive for wet processing). Diffusion bonding of like and unlike ceramics with the aid of a liquid phase.

CORNING GLASS WORKS
Sullivan Park
Corning, NY 14830

344. LUMINESCENT GLASS-CERAMICS: OPTICAL SPECTROSCOPIC INVESTIGATIONS

G. H. Beall
Research and Development Div.
Phone: (607) 974-3430

$189,800 02-2

Compositional studies of doped glass-ceramics with potentially useful luminescent behavior. Preparation and characterization of transparent host compounds based on various solid solution crystals and doped with transition metal and rare earth luminescing ions. Properties of interest: nucleating agents, crystallinity, particle size, optical perfection, thermal expansion, and refractive index. Spectroscopic properties, radiative transfer and glass-ceramic structure evaluated from measurements of absorption, emission and excitation spectra, fluorescence yield, excited-state lifetimes, light scattering, and electron paramagnetic resonance.

DARTMOUTH COLLEGE
Hanover, NH 03755

345. THE STRUCTURE AND MECHANICAL PROPERTIES OF STOICHIOMETRIC NI_3AL AND OF NI3AL ALLOYED WITH BORON

E. M. Schulson
Thayer School of Engineering
Phone: (603) 646-2888

$107,540 01-2

Structure and mechanical properties of stoichiometric Ni_3Al and of Ni_3Al microalloyed with 750ppm boron consolidated from rapidly solidified powders via two and three-stage hot and warm extrusion. Correlation of discontinuous yielding, yield strength, work hardening, ductility and fracture mode in tension (at 77 to 1023 K) with grain size, superlattice dislocations and superlattice faults. Microstructural stability, dynamic recrystallization. Use of conventional and analytical TEM for microstructural examination, XRD for texture determination, SEM-SACP's for fractography and AES for segregation to grain boundaries.

UNIVERSITY OF DELAWARE
Newark, DE 19716

346. DURABILITY OF SHORT FIBER COMPOSITE MATERIALS

T.-W. Chou
Dept. of Mechanical and Aerospace Engineering
Phone: (302) 451-2904

$49,742 01-2

Experimental and theoretical investigaton 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.

347. NEUTRON STUDIES OF LIQUID AND SOLID HELIUM

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

$67,000 02-3

Theoretical calculation of properties of liquid and solid helium for direct comparison with neutron measurements. Aim to interpret neutron scattering experiments, investigate the consequences of experiments in terms of existing and new models and to propose new experiments. Specific examples: direct calculation of the dynamic form factor $S(Q,\omega)$ in liquid ^3He for comparison with existing data in order to test models of the effective interaction between the atoms in the liquid, calculations of the momentum distribution in liquid ^3He and solid ^4He for comparison with measurements at IPNS (ANL), and to test the impulse approximation using models appropriate to solid ^4He.

UNIVERSITY OF DENVER
Denver, CO 80208

348. CATION DOPANT EFFECTS ON THE LATTICE THERMAL EXPANSION OF CORDIERITE

P. K. Predecki
Dept. of Chemistry
Phone: (303) 753-2141

$84,908 01-3

Lattice thermal expansion measurements on cordierite doped with alkali and alkaline earth dopants using high-temperature Guinier X-ray diffractometry. Neutron powder diffraction studies at the IPNS at ANL. Reitveld structure refinement of neutron diffraction data to provide atom positions, site occupancies, and anisotropic temperature factors.

349. DETECTING AND MONITORING CRACK INITIATION AND GROWTH IN AUSTENISTIC AND FERRITIC STEELS

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

$61,405 01-5

Experimental investigation of new techniques to study the initiation and growth of cracks in hydrogen environment, techniques include continuous measurement of elastic modulus and acoustic emission, materials investigated include pure iron and a number of stainless steels, measurements are carried out at zero load as well as under applied stress, additional measurements of the internal friction provide insight and information on hydrogen-dislocation interactions, acoustic emission tests on small pressure vessels to determine if acoustic emission monitoring can be used on real structure exposed to hydrogen environments.

FLORIDA STATE UNIVERSITY
Tallahasee, FL 32306

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

J. G. Skofronik
Dept. of Physics
Phone: (904) 644-5497
S. A. Safron
Dept. of Chemistry
Phone: (904) 644-5239

$200,000 02-2

Study of the dynamics of surfaces by the scattering of low energy He atoms. Measurement of phonon lifetimes analyzed for important information concerning relaxation phenomena. Studies include: The behavior of the (110) surfaces of Au, Pt, and Ir which reconstruct as a function of temperature, the surfaces of active metals such as Ni and Cu, including measurements on physisorbed and chemisorbed layers. Study of phonon anomalies of surfaces in high Tc superconducting materials, both 3-d and 4-d, and of layered compounds such as $TaSe_2$ and $NbSe_2$, in which charge density wave (CDW) form at low temperatures.

UNIVERSITY OF FLORIDA
Gainesville, FL 32611

351. MODERATE AND LOW TEMPERATURE OXIDATION OF CLEAN NICKEL, CHROMIUM, AND NI-CR ALLOYS

P. Holloway
Dept. of Materials Science and Engineering
Phone: (904) 392-6664
C. Batich
Dept. of Materials Science and Engineering
Phone: (904) 392-6630

$117,948 01-3

Investigation of low and moderate temperature (100 $K^{o} < T < 800^{o}K$) 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.

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

J. J. Hren
Dept. of Materials Science and Engineering
Phone: (904) 392-6985

$5,500 01-3

Investigation of hydrogen trapping sites and diffusion in BCC and FCC metals (Nb and Ni, respectively) using TEM and field ion microscopy, pulse desorption to determine trap site energetics, influence of substitutional solutes on above. Implantation of D and He into Ni and Fe emitters at energies up to 20 keV. Characterization of emitters by transmission electron microscopy before and after implantations. Coupling of ion source to imaging atom probe for <u>in situ</u> implantation at ~40-50 K followed by IAP analyses.

UNIVERSITY OF FLORIDA (continued)

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

M. D. Sacks
Dept. of Materials Science and Engineering
Phone: (904) 392-6676
J. W. Williams
Dept. of Materials Science and Engineering
Phone: (904) 392-6698
C. D. Batich
Dept. of Materials Science and Engineering
Phone: (904) 392-6630

$120,000 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.

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

T. E. Hogen-Esch
Dept. of Chemistry
Phone: (904) 392-2011
G. B. Butler
Dept. of Chemistry
Phone: (904) 392-2012

$98,000 03-1

Study of graft copolymerization of vinyl monomers to polysaccharides to determine grafting efficiencies and the structure and properties of the copolymers. A variety of model polymers will be synthesized which contain the specific reactive functional groups of the polysaccharide repeating unit, possess controlled branching sites, and contain macrocyclic units to aid in establishing viscosity-stucture relationships. Also extensive characterization and rheological studies will be undertaken with the purpose of developing novel methods for characterization of high-molecular-weight, water-soluble polymers, when necessary.

GEORGIA INSTITUTE OF TECHNOLOGY
Atlanta, GA 30332

355. THE STRUCTURE AND REACTIVITY OF HETEROGENEOUS SURFACES AND STUDY OF THE GEOMETRY OF SURFACE COMPLEXES

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

$167,000 02-3

Theoretical studies to provide a coherent understanding of the fundamental processes which underly and control the structure, transformations, growth, processing electronic properties and reactivity of materials and material surfaces. Analytical methods and novel numerical simulation (molecular dynamics) techniques developed and employed in investigations of phase transformations, solidification, laser annealing, defect formation, energetics and dynamics of transport phenomena, stability and reactivity of systems relevant to energy technologies.

356. A CARBANION APPROACH TO POLYACETYLENE

L. M. Tolbert
Dept. of Chemistry
Phone: (404) 894-4003

$71,542 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.

HARVARD UNIVERSITY
Cambridge, MA 02138

357. 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.

358. FUNDAMENTAL PROPERTIES OF SPIN-POLARIZED QUANTUM SYSTEMS

I. F. Silvera
Dept. of Physics
Phone: (617) 495-9078, 2872

$209,997 (11 Months) 02-2

Investigation of the properties of the quantum gases of spin-polarized atomic hydrogen and deuterium. Attempt to reach high enough densities and low enough temperature that these unusual gases undergo Einstein-Bose Condensation. If this new form of matter obtained, the expected superfluidity of this weakly interacting gas is to be sought and, if found, characterized.

UNIVERSITY OF ILLINOIS/CHICAGO CIRCLE
Chicago, IL 60680

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

M. McNallan
Dept. of Civil Engineering, Mechanics and Metallurgy
Phone: (312) 996-2436

$35,882 01-3

Experimental investigation of the oxidation of transition metals (Fe, Ni, Co) in mixed gas environments containing oxygen and chlorine. Thermogravimetric measurement of corrosion kinetics. Analysis of corrosion product morphologies and chemistries using optical and electron microscopy. Interpretation of corrosion mechanisms in mixed gas environments containing volatile corrosion products and characterization of corrosion kinetics under these conditions. Behavior described in terms of chlorination, paralinear oxidation, or catastrophic oxidation. Identification of thermodynamic conditions producing latter behavior in each metal.

INDIANA UNIVERSITY
Bloomington, IN 47402

360. HIGH-RESOLUTION ELECTRON ENERGY LOSS STUDIES OF SURFACE VIBRATIONS

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

$82,896 (15 Months) 02-2

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.

UNIVERSITY OF KENTUCKY
Lexington, KY 40506

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

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

$142,000 (15 Months) 02-2

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.

UNIVERSITY OF KENTUCKY (continued)

362. STRUCTURAL 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

$84,989 03-3

Structural and morphological studies on small metal crystallites dispersed in porous support phases, influence of interactions between metal and support, metals include nickel, gold, and cobalt, support phases include silica, magnesium silicate, and nylon. Techniques used: analytical electron microscopy, X-ray diffraction, ion scattering spectroscopy, energy dispersive X-ray analysis, and microdiffraction.

LEHIGH UNIVERSITY
Bethlehem, PA 18015

363. 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 01-1

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_2O_3-La_2O_3 system. Precipitate coarsening kinetics in NiO and CoO, and precipitation processes in mullite and glass ceramic materials.

LEHIGH UNIVERSITY (contined)

364. 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.

365. CORROSION FATIGUE OF SMALL CRACKS: MECHANICS AND CHEMISTRY

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

$90,650 (7 Months) 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, modelling of electrochemical conditions near the crack tip and of the electrochemical and micromechanics aspects of small-crack growth.

UNIVERSITY OF MARYLAND
College Park, MD 20742

366. 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

$202,595 02-2

Joint theoretical/experimental investigation of surface interactions and imperfections which have an important influence on surface reactivity. Studies of oxygen adsorption and reaction at low temperatures on polycrystalline films and single crystal surfaces. Measurements of adatom-adatom interactions with high resolution LEED/Auger to examine the degree of 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.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
Cambridge, MA 02139

367. 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

$328,400 01-1

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.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

368. 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

$305,000 (6 Months) 01-1

Electrical and optical behavior of Al_2O_3 and MgO, including vacuum ultraviolet spectroscopy characterization of band gaps. Float zone laser crystal growth and zone refining in Al_2O_3 and grain boundary migration in high purity powder and bicrystals of Al_2O_3. 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 $SrTiO_3$, and Bi and O grain boundary diffusion in ZnO. Defect structures, defect interaction, grain boundary and surface studies include 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 Al_2O_3, 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 $SrTiO_3$, and role of grain boundary segregation on high temperature deformation in SiC and Al_2O_3. 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 Al_2O_3, and orientation effects on the grain boundary migration of high purity Al_2O_3.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

369. 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

$75,020 (5 Months) 01-2

Development of constitutive flow relations for transformation plasticity based on nucleation-controlled martensitic transformation kinetics in both homogeneous and dispersed-phase composite materials, critical experiments on specially-designed model materials in metals (high-strength austenitic and martensitic steels), ceramics (ZrO_2 and alkali halide dispersed-phase composites), and metallic glasses, influence of stress-state, strain-rate, and temperature, determination of nucleation site potency distributions and influence on flow behavior, TEM study of nucleation in ZrO_2 small-particle bicrystals, application of constitutive relations in crack-tip plasticity calculations as a basis for toughening.

370. RAPIDLY SOLIDIFIED CERAMICS

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

$112,800 01-3

Rapid solidification studies of the systems Al_2O_3-ZrO_2, Al_2O_3-MgO, Y_2O_3-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.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

371. BASIC MECHANISMS OF THE OXIDATION OF METALS AND ALLOYS

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

$165,000 01-3

Effects of temperature and oxygen partial pressure on the kinetics of growth of Cr_2O_3 scales on pure Cr and Fe-Cr alloys. Defect structure and diffusion mechanisms in Cr_2O_3 scales. Effect of oxide grain growth on the kinetics of growth of oxide scales. Early stages of the oxidation/sulfidation of Cr and Fe-Cr alloys in H_2-H_2O-H_2S gas mixtures. Factors controlling the transition for nonprotective to protective scaling of alloys in sulfur-bearing environments. Oxidation behavior of polycrystalline, rapidly solidified Fe-Cr-Si and Fe-Cr-Ni-Si alloys. Oxidation kinetics determined by thermogravimetry. Characterization of alloys and scales by SEM, TEM/STEM, EPMA, AES/ESCA and XRD.

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

L. W. Hobbs
Dept. of Materials and Engineering
Phone: (617) 253-6835

$144,026 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, $MgO.nAl_2O_3$, CaF_2, PuO_2, ZrO_2, SiC, Si_3N_4, Li_2O, $LiAlO_2$, $LiAl_5O_8$, Li_2ZrO_3, $Ca(Zr,Pu)Ti_2O_7$, titan SiO, GeO, $ZrSiO_4$. Neutron, ion and electron irradiation damage will be studied, including the effects of massive recoil nuclei and fission fragments.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

373. PHYSICS AND CHEMISTRY OF PACKING FINE CERAMIC POWDERS

H. K. Bowen
Dept. of Materials Science and Engineering
Phone: (617) 253-6892

$125,015 01-5

Development of a scientific basis for the processing and packing behavior of the model sub-micron ceramic powders SiO_2, TiO_2, and SiC. Synthesis aspects of the colloid chemistry and mono-sized particle masses. Colloid coagulation. Surface chemistry and powder characterization. Ordering behavior of particulate assemblies. Effects of particle size distribution on slurry stability. Dispersion, packing, and sintering behavior. Generalizations controlling the presintered structure of compacts containing 10^{12} particles. Laser diffraction. Photon correlation spectroscopy.

374. LOW TEMPERATURE AND NEUTRON PHYSICS STUDIES

C. G. Shull
Dept. of Physics
Phone: (617) 253-4812

$318,970 02-1

Experimental studies of the possible existence of a magnetic monopole charge on the neutron using a technique which exploits the very small effective-mass property of neutrons in a diffracting crystal. Continuing investigations of the piezoelectric strain constant in quartz, of magnetic focusing of neutrons by shaped magnetic fields, and on the anomalous Borrmann transmission in crystals.

375. BASIC STUDIES OF SUBMICRON LAYERS OF Nb-Al

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

$110,365 02-2

Basic studies of model layered structures of Nb and Al to understand the fundamental properties of low temperature reacted Nb-Al. Bilayers and multilayers of Nb and Al used in study the effects of layer structures, oxygen, third element additives, proximity, and mechanisms for high critical currents in thin layers. Model systems to approach actual systems produced by coextrusion of foil materials and powder processed techniques. Investigation of other Nb_3X materials such as Nb_3Ge, Nb_3Ga and $Nb_3(AlGe)$ to determine whether the results for Nb-Al are extendable to these materials and in the search for materials with higher transition temperatures and critical fields.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

376. 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) 253-5578

$140,000 02-2

Attempt to improve critical field of A15 V_3Ga (present best value about 25T) by increasing spin-orbit scattering by inclusion of high Z elements. Two approaches: the inclusion of randomly placed high Z elements with minimum lattice distortion and thin closely spaced high Z material layers. Samples prepared by electron beam evaporation and characterized by the superconducting properties, resistivity and spin-polarized tunneling measurements. These measurements to test existing theoretical concepts and to advance the understanding of high field superconductors as well as the role of many-body effects in normal transition metal systems and the development of improved magnetic solenoids.

MICHIGAN STATE UNIVERSITY
East Lansing, MI 48823

377. DYNAMIC RECRYSTALLIZATION DURING HIGH TEMPERATURE LOW CYCLE FATIGUE OF NICKEL

G. Gottstein
Dept. of Metallurgy, Mechanics, and Materials Science
Phone: (517) 353-9767

$54,683 01-2

Investigation to establish the conditions, limits, and criteria for the occurrence of dynamic recrystallization and its impact on materials performance during low cycle fatigue of Ni and Ni_3Al. Analysis of dislocation structure, subboundary misorientation and internal stresses at subboundary joints. Correlation of dislocation substructure and dynamic recovery kinetics with nucleation of dynamic recrystallization. Dependence and impact of dynamic recrystallization on strain localization, crack nucleation and crack growth. Development and control of dynamically recrystallized structure, grain size and texture. Characterization techniques include mechanical testing, TEM, and STEM, X-ray pole figure measurements and X-ray micro-Laue diffraction.

MICHIGAN TECHNOLOGICAL UNIVERSITY
Houghton, MI 49931

378. ENVIRONMENT-INDUCED EMBRITTLEMENT: EFFECTS OF IMPURITY SEGREGATION AND STATE OF STRESS

L. A. Heldt
Dept. of Metallurgical Eng.
Phone: (906) 487-2630
D. A. Koss
Dept. of Metallurgical Eng.
Phone: (906) 487-2170

$94,000 01-2

Hydrogen embrittlement and stress corrosion cracking with concern for the effects of (1) intergranular misorientation and segregation, and segregant state, (2) stress state and mode of deformation, (3) local chemistry variation, and (4) electrochemistry and temperature. Experimental methods include (1) multiaxial deformation and fracture testing, (2) Auger electron and X-ray photoelectron spectrometry, (3) crack initiation and propagation studies, and (4) bicrystal testing.

379. 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.

UNIVERSITY OF MICHIGAN
Ann Arbor, MI 48109

380. EFFECT OF MICROSTRUCTURE ON THE MECHANICAL PROPERTIES OF SILICON NITRIDE CERAMICS

T. Y. Tien
Dept. of Materials & Metallurgical Engineering
Phone: (313) 764-9449, 7489

$96,540 01-1

Study of role and mechanism of nucleating agents on the crystallization of the Si_2N_2O containing boundary phases which are formed during the processing of Si_3N_4 (containing Y_2O_3 and Al_2O_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.

381. A SYSTEMATIC APPROACH TO INTERGRANULAR CRACKING MECHANISMS IN AUSTENITIC ALLOYS THROUGH GRAIN BOUNDARY CHEMISTRY CONTROL

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

$92,189 01-2

Determination of the role of grain boundary chemistry, chromium depletion, carbide precipitation and phosphorous segregation, taken individually and collectively, on intergranular corrosion, stress corrosion cracking and hydrogen embrittlement of P and C doped Ni-Cr-Fe alloys. Grain boundary composition (Cr and P) and carbide distribution monitored by STEM and AES. Corrosion testing techniques, potentiodynamic polarization scans, electrochemical potentiokinetic reactivation and constant extension rate testing.

382. SURFACE-PLASMON EXPLORATION OF MULTILAYER PHYSISORBED AND CHEMISORBED FILMS ON METAL SUBSTRATES

M. Bretz
Dept. of Physics
Phone: (313) 764-4494

$75,000 02-2

Measurement of dielectric properties of adsorbed films by laser excitation of surface plasmons. Technique permits study of phase transitions in monolayer to multilayer films following layer-by-layer evolution of films from two to three dimensions, detection of orientational effects of non-spherical adsorbed molecules, and study of a variety of other surface phenomena.

UNIVERSITY OF MICHIGAN (continued)

383. GROWTH AND DYNAMICS OF SCALE INVARIANT MATTER

L. M. Sander
Dept. of Physics
Phone: (313) 764-4471
R. Savit
Dept. of Physics
Phone: (313) 764-3426

$71,525 (8 Months) 02-3

Study of relationships between growth mechanisms, structure, and properties of non-equilibrium systems, such as smoke, colloids, and electrolytic depositions, which have scale invariant fractal-like structures. Objects of this type have a morphology which lies between the conventionally studied crystalline geometry (with a very high degreee of regular symmetry) and the amorphous state (with no special symmetry). Development of a mathematical description of growth process and caluclation of long-distance structures and dynamics of the resulting structures.

UNIVERSITY OF MINNESOTA
Minneapolis, MN 55104

384. 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

$776,217 (8 Months) 01-1

Basic research and technology transfer in corrosion. Electron transfer at solid-electrolyte interface and capacitance. In situ IR spectroscopy at the solid-liquid interface. Study of passivating films by inelastic electron tunneling spectroscopy, rotating ring-disc electrode, electrochemical oscillations, and their destruction by mechanical and chemical effects. Photoelectrochemistry and electrochemical oscillation, and their destruction by mechanical and chemical effects. Photoelectrochemistry and electroluminescence of oxides. Dissolution kinetics of oxide films. Surface microtopography and corrosion of GaAs. Cathodic reduction of hydrogen. Corrosion protection by conducting organic polymers. In situ measurement of stresses in oxide scales by energy dispersive X-ray diffraction, and of their relaxation by acoustic emission. Mechanism of break-down of oxide coatings in relation to parameters.

UNIVERSITY OF MINNESOTA (continued)

385. 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

$50,576 (6 Months) 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 and Fe-Ni 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 analyse near-surface deformation.

386. 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 AT KANSAS CITY
1110 E. 48th Street
Kansas City, MO 64110

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

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

$72,848 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.

UNIVERSITY OF MISSOURI
Columbia, MO 65211

388. MEASUREMENTS TO VERIFY BRAGG DIFFRACTION AND TOTAL REFLECTION AT A NARROW NUCLEAR RESONANCE

R. M. Brugger
Research Reactor Facility
Phone: (314) 882-4211

$76,996 (24 Months) 02-1

Measurement of resonance Bragg diffraction of neutrons of several important isotopes that have potential use at pulsed spallation neutron sources. A search for crystals suitable as monochromators and filter detectors. Studies of total reflection at resonance for a few selected isotopes for use as neutron mirrors in the epithermal region.

UNIVERSITY OF MISSOURI AT COLUMBIA (continued)

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

H. R. Chandrasekhar
Physics Department
Phone: (314) 882-6086

$48,051 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.

390. 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 science experiments using the unique source of Tungsten-183 with 46.5 keV Mossbauer radiation at the University of Missouri, intensity about one thousand times more intense than that used in most Mossbauer Spectroscopy experiments. A special Microscopic Conversion Electron (MICE) detector developed and now used. Experiments to separate the elastic and inelastic scattering at Bragg reflections, to determine the quasielastic linewidths observed in critical phenomena, and to study very low energy Landau excitations will be undertaken. In collaboration with J. G. Mullen at Purdue.

UNIVERSITY OF MISSOURI (continued)

391. CHARACTERIZATION OF THE REDOX BEHAVIOR AND STABILITY OF ELECTRICALLY CONDUCTING OXIDES

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

$123,000 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.

UNIVERSITY OF NEVADA
Reno, NV 89557

392. INVESTIGATIONS OF TRIPLET EXCITON PROCESSES OCCURRING IN PURE POLYMERFILMS

R. D. Burkhart
Dept. of Chemistry
Phone: (702) 784-6041

$85,000 03-1

Determination of the speed and migratory range of triplet excitons in pure polymer films. The work involves the development of experimental methods and the preparation of suitable polymer substrates.

UNIVERSITY OF NEW MEXICO
Albuquerque, NM 87131

393. RADIATION EFFECTS AND ANNEALING KINETICS IN CRYSTALLINE COMPLEX NB-TA-TI OXIDES, PHOSPHATES, AND SILICATES

R. C. Ewing
Geology Dept. of Geology
Phone: (505) 277-4163

$75,000 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.

NEW YORK UNIVERSITY
4 Washington Place
New York, NY 10003

394. PHOTOEMISSION STUDIES OF F-ELECTRON SYSTEMS: MANY BODY EFFECTS

R. D. Parks
Dept. of Physics
Phone: (212) 598-2600

$90,000 02-2

Photoemission studies using ultraviolet, X-ray and synchrotron radiation stimulation to understand the 4f instability in the early rare earths and the localized versus itinerant behavior of the 5f electrons in the early actinides. Related studies of the effect of substrate on the valence of ytterbium adatoms and of surface valence shifts and reconstruction in 4f-unstable rare-earth-based systems. Synchrotron-radiation-stimulated photoemission studies are performed at National Synchrotron Light Source.

POLYTECHNIC INSTITUTE OF NEW YORK
333 Jay Street
Brooklyn, NY 11201

395. MIXED VALENT BEHAVIOR IN ACTINIDES AND RELATIONSHIP TO CERIUM

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

$106,667 (18 Months) 02-3

Theoretical research on the many body aspects of materials containing the early actinide elements and Ce. Principal subjects: 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. The basic theoretical model: a lattice of magnetic ions (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. The role of electron phonon-mediated couplings and other possible exotic coupling mechanisms in the heavy fermion superconductors $CeCu_2Si_2$, UBe_{13} and UPt_3.

396. LOCAL MANY-BODY EFFECTS IN THE OPTICAL RESPONSE OF NARROW BAND SOLIDS

A. Zangwill
Dept. of Physics
Phone: (212) 643-2190
D. Liberman
Lawrence Livermore National Laboratory

$57,613 (16 Months) 02-3

Provide realistic calculations of expected photoelectric partial cross sections for the late 3d transition metals, cerium, the light actinides and the associated intermetallic compounds of all the aforementioned. Such calculations to provide essential guidance in interpretation of experiments involving photoabsorption and photoemission measurements in the vicinity of near core and deep core thresholds. Calculation from RPA-type theory based on the density functional formalism applied to an embedded cluster model of condensed matter. Special care will be taken to simulate the interplay between dielectric and core-hole many-body effects, both of which are expected to be important in the materials of interest.

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

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

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

$105,063 01-1

Preparation of thin-film surface coatings by glow discharge and reactive sputtering of disordered alloys of carbon, silicon, and hydrogen ($C_xSi_yH_z$) 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.

398. DYNAMICS OF FLUID SURFACES AND THE CRYSTAL-MELT INTERFACE

H. Z. Cummins
Dept. of Physics
Phone: (212) 690-6921

$150,640 (18 Months) 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.

CITY UNIVERSITY OF NEW YORK/CITY COLLEGE (continued)

399. MAGNETIC PROPERTIES OF DOPED SEMICONDUCTORS

M. Sarachik
Dept. of Physics
Phone: (212) 640-8206

$33,608 (3 Months) 02-2

This is to be a systematic, precise, and careful 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. The measurements made with a Faraday balance, both as a function of temperature (from 1.25 K to 300 K) and as a function of magnetic field (to 50 kG) to separate various contributions to the total susceptibility. The measurements extended to 50 mK and 190 kG at the National Magnet Laboratory. To ascertain whether percolation plays a role in the transition by determining whether a contribution associated with conduction electrons (or holes) persists into the insulating range of concentration.

400. ELECTRONIC AND OPTICAL PROPERTIES OF DISORDERED SYSTEMS

M. Lax
Dept. of Physics
Phone: (212) 690-6864, (201) 582-6527

$91,147 (16 Months) 02-3

An extensive theoretical study of transport and optical properties of disordered media such as amorphous materials, doped semiconductors, quasi-one dimensional conductors, and interfaces, etc.

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

401. X-RAY TOPOGRAPHY PRT ON LINE X-19 AT NSLS

J. C. Bilello
Dept. of Materials Science
Phone: (516) 246-5983

$500,000 01-1

Development of facilities for X-ray topography at the National Synchrotron Light Source (NSLS) and implementation of advanced materials research. Research includes studies of hydride precipitation in the niobium-hydrogen system, investigation of high temperature grain boundary failure mechanisms, fundamental studies on crack initiation and propagation in elastic-plastic materials, thermal decomposition mechanisms in inorganic single crystals, internal stresses in protective coatings for fusion applications, morphology of CdS after pressure quenching, characterization of strains and effects in metal-silicide thin films on Si substrates and direct measurements of the interaction of acoustic waves in solids with the microstructure.
The members of the Participating Research Team (PRT) for X-ray topography include Prof. J. Bilello (Project Director), Profs. H. Birnbaum and H. Chen (Univ. of Illinois), Prof. R. Green (Johns Hopkins Univ.), Profs. P. Herley and H. Herman (Stony Brook), Prof. D. Pope (Univ. of Pennsylvania), Prof. R. MacCrone (RPI), Drs. M. Suenaga, J. Hastings and W. Thomlinson (BNL), and Dr. J. Patel (Bell Laboratories, Murray Hill). Associated Users include Drs. D. Davidson (Southwest Research Institue), S. Stock (Northwestern Univ.), and S. Weissman (Rutgers Univ.).

402. INTERFACE PROPERTIES AND CRYSTAL-GROWTH

J. Q. Broughton
Dept. of Materials Science and Engineering
Phone: (516) 246-6759, 6754

$119,147 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.

STATE UNIVERSITY OF NEW YORK/STONY BROOK (continued)

403. OPERATION, MAINTENANCE AND UPGRADING OF SUNY PRT FACILITIES AT THE NATIONAL SYNCHROTRON LIGHT SOURCE

J. Bigeleisen
Dept. of Chemistry
Phone: (516) 246-7945

$400,000 02-2

Development and operation of an X-ray beam line at NSLS by the SUNY Participating Research Team (PRT). The facilities include instrumentation for high-resolution crystallography, surface science, small angle X-ray scattering (SAXS), and Extended X-ray Absorption Fine Structure (EXAFS). The PRT represents campuses at Albany, Buffalo, Stony Brook, Cortland, and Alfred and has Allied Corporation as an industrial participant.

404. SURFACE STUDIES BY A VUV PRT AT THE NATIONAL SYNCHROTRON LIGHT SOURCE

F. Jona
Dept. of Materials Science and Engineering
Phone: (516) 246-7649, 6759

$150,000 02-2

Development of a versatile, high-vacuum experimental chamber for surface research with the VUV ring at NSLS with LEED, Auger, SEXAFS, and photoemission facilities. Studies of atomic structure of solid surfaces: Al, Fe, and Ti, both clean and with O, S, Cl, and CO adsorbates. Chemisorption, physisorption and hydrogen uptake: H uptake by Nb, O on Ni and Nb, Pd on Nb and Ta. Electronic properties of solids: lifetimes of excited states in metals and insulators, effects of bulk phase transitions on surface structure, surface and bulk properties of FeTi.

STATE UNIVERSITY OF NEW YORK/STONY BROOK (continued)

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

J. L. Whitten
Dept. of Chemistry
Phone: (516) 246-6068

$124,000 03-3

Theoretical study of the structure and energetics of molecules adsorbed on solid surfaces and dissociative chemiadsorption with emphasis on transition metal substrates. The primary emphasis of the work is on the energetics of adsorption as a function of surface site and composition, with the objective of determining the reactivity of adsorbed species. Theoretical work will focus on the accurate treatment of electronic interactions, the configuration interaction description of closely spaced Ni states and changes in states during chemiadsorption, and on the representation of fields acting the embedded electronic subspace.

NORTH CAROLINA AGRICULTURAL & TECH. UNIV
Greensboro, NC 27411

406. 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

$65,000 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.

NORTH CAROLINA CENTRAL UNIVERSITY
Durham, NC 27707

407. 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_3N_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.

NORTH CAROLINA STATE UNIVERSITY
Raleigh, NC 27650

408. MICROSTRUCTURAL EFFECTS IN SOLID PARTICLE EROSION

R.O. Scattergood
Dept. of Materials Engineering
Phone: (919) 737-2377
H. Conrad
Dept. of Materials Engineering
Phone: (919) 737-2377

$92,610 01-5

Correlation of erosion rates in multiphase systems with constituent phase properties and distribution. Systems under investigation: Al-Si alloys, WC-Co cermets and alumina-stainless steel composites. 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. Constituitive and averaging laws for erosion rates to be developed from experimental results and modeling/computer simulation.

NORTH CAROLINA STATE UNIVERSITY (continued)

409. 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

$275,000 02-2

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

NORTHEASTERN UNIVERSITY
Boston, MA 02115

410. POSITRON STUDIES OF DEFECTED METALS AND METALLIC SURFACES

Arun Bansil
Dept. of Physics
Phone: (617) 437-2902

$102,000 (16 Months) 02-2

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.

NORTHWESTERN UNIVERSITY
Evanston, IL 60201

411. ELECTRONIC AND STRUCTURAL PROPERTIES OF SEMICONDUCTOR HETEROJUNCTIONS

Y. W. Chung
Dept. of Materials Science and Engineering
Phone: (312) 492-3112

$43,395 01-1

Comprehensive investigation of α-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.

412. POINT DEFECT CLUSTERS AND ELECTRICAL BEHAVIOR IN TRANSITION METAL OXIDES

J. B. Cohen
Dept. of Materials Science and Engineering
Phone: (312) 492-3570
D. E. Ellis
Dept. of Physics and Astronomy
Phone: (312) 492-3665
T. O. Mason
Dept. of Materials Science and Engineering
Phone: (312) 492-3198

$170,149 01-1

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_3O_4, $CoAl_2O_4$, and $FeAl_2O_4$.

NORTHWESTERN UNIVERSITY (continued)

413. AN INVESTIGATION OF MICROSTRUCTURAL CHANGES IN FERRITIC STAINLESS STEELS CAUSED BY HIGH TEMPERATURE DEFORMATION

J. R. Weertman
Dept. of Materials Science and Engineering
Phone: (312) 492-5393

$75,800 01-2

Investigation of deformation, failure, and microstructural stability during creep and creep fatigue in ferritic stainless steels, influence of thermal and mechanical history, environment, and alloy composition on mechanical properties, HVEM and SANS characterization of strain and thermal induced microstructural modifications. e.g., carbide precipitation, dislocation structures, cavity formation.

414. DEFECT STRUCTURE OF SEMICONDUCTING AND INSULATING OXIDES

B. W. Wessels
Dept. of Materials Science and Engineering
Phone: (312) 492-3219

$73,020 01-3

Use of space charge spectroscopy techniques to explore the deep level 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 $SrTiO_3$.

NORTHWESTERN UNIVERSITY (continued)

415. STRUCTURAL AND FAST ION TRANSPORT PROPERTIES

D. H. Whitmore
Dept. of Materials Science and Engineering
Phone: (312) 492-3533
P. Georgopoulos
Dept. of Materials Science and Engineering
Phone: (312) 492-3533

$111,000 01-3

Detailed structural and ionic transport studies of fast ion conducting glasses including mixed valence, proton conducting and selenide based glasses and amorphous polyphosphazine 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.

416. 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) 492-3685, 3644
A. Gonis
Dept. of Physics and Astronomy

$73,000 02-3

Determination of the thermodynamic properties and short-range-order parameters of ordered and substitutionally disordered alloys from ab-initio all-electron calculations taking into account the lattice structure, statistical fluctuations and utilizing fully relativistic energy band programs. Recently developed theoretical and computational methods based on local density theory and a cluster generalization of the coherent potential approximation used to obtain the density of states. These calculations to identify multi-site potentials to be used with existing theories, such as the cluster variational method of Kikuchi, to construct alloy phase diagrams.

NORTHWESTERN UNIVERSITY (continued)

417. INTERFACIAL ELECTRICAL TRANSPORT IN BATTERIES EMPLOYING SOLID ELECTROLYTES

M. Ratner
Dept. of Chemistry
Phone: (312) 492-5652
D. Shriver
Dept. of Chemistry
Phone: (312) 492-5655

$84,675 03-2

Investigation of ionic transport along and through interfaces, both within a given solid electrode or electrolyte and between solid electrodes and electrolytes. The objective is mechanistic understanding of which processes result in overpotential, degradation, charge buildup, and enhanced mobility at such interfaces. Two general classes of materials will be investigated: polyether solid electrolytes and insertion cathodes. Experiments will include preparation, surface modification, electrochemical and spectroscopic characterization, and a. c. conductivity. Theoretical work will involve simulations using Monte-Carlo, Langevin dynamics, and dynamic percolation theory techniques.

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

P. Dutta
Dept. of Physics and Astronomy
Phone: (312) 492-5465
J. B. Ketterson
Dept. of Physics and Astronomy
Phone: (312) 492-3644

$97,717 03-3

Study of the mechanical properties of organic monolayers on the surface of water (Langumuir 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

419. MICROSTRUCTURAL EFFECTS IN ABRASIVE WEAR

T. H. Kosel
Dept. of Metallurgical Engineering and Materials Science
Phone: (219) 239-5642

$75,052 01-5

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

420. 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

$74,958 01-1

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

OHIO STATE UNIVERSITY (continued)

421. FUNDAMENTAL STUDIES OF HIGH TEMPERATURE CORROSION REACTIONS

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

$78,867 01-1

In situ SEM study of oxidation of metals, Fe, Ni, Cu and Cr, and binary alloys of these metals, effect of H_2 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 Fe_2O_3 and whiskers in NiO.

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

P. G. Shewmon
Dept. of Metallurgical Engineering
Phone: (614) 422-2491

$69,775 01-2

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.

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

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

$106,401 01-5

Experimental and analytical research to study interactions of ultrasonic waves with boundaries separating anisotropic materials. Single crystals of nickel prepared and diffusion bonded to both polycrystalline and other single crystals. Computer controlled ultrasonic parameters in the crystals and at the boundaries. Analysis of energy transport and wave partitioning.

OREGON STATE UNIVERSITY
Corvallis, OR 97331

424. PERTURBED ANGULAR CORRELATIONS IN ZR-CONTAINING CERAMICS

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

$67,217 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_2O_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.

PENNSYLVANIA STATE UNIVERSITY
University Park, PA 16802

425. PHYSICAL CHEMISTRY OF PORTLAND-CEMENT HYDRATE, RADIOACTIVE WASTE-HOSTS

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

$61,621 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.

PENNSYLVANIA STATE UNIVERSITY (continued)

426. VIBRATIONAL AND OPTICAL STUDIES OF AMORPHOUS METALS

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

$86,940 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.

427. SPECTROSCOPIC INVESTIGATIONS OF GLASS STRUCTURE

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

$118,000 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.

PENNSYLVANIA STATE UNIVERSITY (continued)

428. TWIN BOUNDARIES AND HETEROPHASE INTERFACES IN FERROELASTIC MARTENSITES

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

$150,000 01-3

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 of $In_{1-x}Tl_x$ 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.

429. GRAIN BOUNDARY AND SURFACE DIFFUSION IN OXIDE SYSTEMS

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

$57,500 01-3

Grain boundary impurity diffusion in ionic materials, specifically isotopes of Cr and Fe in Fe_3O_4, influence of point defects on the grain boundary diffusion. Chemistry of grain boundaries. Surface diffusion in oxide materials, specifically isotope of Cr on surfaces of MgO, Al_2O_3, and NiO or isotopes of Cr and Co on CoO surface. Chemistry of surfaces. Techniques used: gamma-rays counting, SIMS, Auger, LEED.

PENNSYLVANIA STATE UNIVERSITY (continued)

430. EXPERIMENTAL AND THEORETICAL STUDIES ON TRANSPORT PROCESSES IN LAZER WELDING

T. DebRoy
Dept. of Materials Science and Engineering
Phone: (814) 865-1974

$41,096 (7 Months) 01-5

Modelling 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.

431. 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 Al_2O_3-SiO_2 compositions around the mullite phase field and Al_2O_3-ZrO_2 both melted with a 10.6 micron CO_2 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.

432. STUDY OF FIELD ADSORPTION USING IMAGING ATOM-PROBE ION MICROSCOPY

T. T. Tsong
Dept. of Physics
Phone: (814) 865-2813

$74,705 02-2

Study in atomic detail of field adsorption of noble gases and classical molecular gases using the imaging atom probe field ion microscope. Measurement of adsorption energy as a function of field on catalytically active group VIII metal surfaces. Mechanism of formation of metal-noble gas complex ions. Photon and electron stimulated field desorption.

PENNSYLVANIA STATE UNIVERSITY (continued)

433. NEW LOW TEMPERATURE (HYDROXYLATED) MATERIALS

R. Roy
Materials Research Laboratory
Phone: (814) 865-3421

$70,000 03-2

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. These materials have potential application as low-level radioactive waste hosts.

UNIVERSITY OF PENNSYLVANIA
Philadelphia, PA 19104

434. ATOMISTIC STUDIES OF THE STRUCTURAL PROPERTIES OF GRAIN BOUNDARIES WITH SUBSTITUTIONAL IMPURITIES

V. Vitek
Dept. of Materials Science and Engineering
Phone: (215) 898-7883

$47,083 01-1

Atomistic computer simulation studies of the structure and properties of grain boundaries containing various concentrations of alloying element, the alloys considered are Cu-Bi, Au-Ag, Cu-Ag, Fe-Sb, Fe-Cu, Fe-Sn. Development of semiempirical scheme for description of interatomic forces in pure metals and alloys in the form of pair potentials and volume dependent term by fitting elastic properties, lattice parameter, cohesive energy, enthalpy of mixing and charge transfers. Relationship between grain boundary structure and propensity to segregation, structural transformations induced by segregation and influence on diffusion, emission and absorption of vacancies and boundary migration, trapping of hydrogen and helium in grain boundaries and their effect on embrittlement.

UNIVERSITY OF PENNSYLVANIA (continued)

435. LOW STRESS BRITTLE FRACTURE IN POLYMERS

N. Brown
Dept. of Materials Science and Engineering
Phone: (215) 898-8506

$51,552 (6 Months) 01-2

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.

436. MECHANISMS OF DAMAGE ACCUMULATION IN TIME-DEPENDENT CYCLIC DEFORMATION

C. Laird
Dept. of Materials Science and Engineering
Phone: (215) 898-8337
J. L. Bassani
Dept. of Mech. Eng. and App. Mechs.
Phone: (215) 898-5632

$112,048 01-2

Identification of microstructural changes resulting from cyclic creep and fatigue deformation of metals, initially Cu and Cr-Mo-V steel, relationship of developing embrittlement of fatigue-induced compositional changes in carbides (Cr-Mo-V), mechanisms of failure in fatigue loading with and without mean loads and its relationships with microstructure, modelling of fatigue-induced property changes, cyclic stress-strain response in the presence of mean loads and its relation to fracture, behavior of single crystals in cyclic creep with special reference to latent hardening, development of effective numerical techniques to model single crystal plasticity by slip, modelling of polycrystalline behavior.

UNIVERSITY OF PENNSYLVANIA (continued)

437. 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.

438. HIGH CONDUCTIVITY PROTON SOLID ELECTROLYTES

G. C. Farrington
Dept. of Materials Science and Engineering
Phone: (215) 898-6642

$87,980 03-1

Preparation and characterization of a series of solid state protonic conductors, for use in the temperature range of 100-400°C. Determination of conductivities of NH_4^+-H^+-β aluminas, and studies of the influence of the stabilizing cation. Studies on single crystals of deuteronium beta and beta" alumina including refinements of atomic positions, band lengths, etc. NMR studies to explore microscopic processes of diffusion.

UNIVERSITY OF PITTSBURGH
Pittsburgh, PA 15261

439. MICROCHEMICAL ANALYSIS F POLYCRYSTALLINE NI AL AND OTHER ORDERED ALLOYS USING THE FIELD-ION ATOM PROBE

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

$113,216 01-1

Investigation of structure and microchemistry of grain boundaries in Ni_3Al 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 a comparison between cast and melt-spun Ni_3Al-B material.

UNIVERSITY OF PITTSBURGH (continued)

440. HIGH TEMPERATURE CORROSION OF CERAMICS

F. S. Pettit
Dept. of Metallurgical and Materials Engineering
Phone: (412) 624-5300

$61,038 01-3

Thermodynamic and kinetic analyses of gaseous and molten salt corrosion of oxides (SiO_2, Al_2O_3, Cr_2O_3, and ZrO_2) in oxidizing, sulfudizing, and reducing environments, thermogravimetric measurement of corrosion kinetics. Gas mixtures of SO_2-SO_3-O_2, H_2-H_2O, and CO-CO_2-O_2 at temperatures in the interval 700° to 1400°C. Effects of deposits such as Na_2SO_4, NaOH and Na_2CO_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.

441. THE PHYSICS OF PATTERN FORMATION AT LIQUID INTERFACES

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

$115,300 (15 Months) 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

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

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

$77,458 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.

443. 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 03-1

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.

PRINCETON UNIVERSITY (continued)

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

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

$90,000 03-1

Reasearch on the relationship between the energy levels of impurity ions and the energy levels in the host crystal. The method to be used is measurement of photoionization thresholds of the impurity ions. The measured values will be used to develop a theoretical description. Included is research on the process of electron ejection into the lattice by acceptor ions. Related research on the local geometry of the crystal in the vicinity of the ion which have lost an electron and the formation of exciplexes is also proposed.

PURDUE UNIVERSITY
West Lafayette, IN 47907

445. NOVEL POLYMERIC LI AND DIVALENT CATION FAST ION CONDUCTING MATERIALS: LI-SALT-IONENIC POLYMER SOLUTIONS, LI CONTAINING PLASTIC,ETC

C. A. Angell
Dept. of Chemistry
Phone: (317) 494-5256
E. I. Cooper
Dept. of Chemistry
Phone: (317) 494-5256

$77,480 01-1

Examination of the possibility of obtaining glasses with a relatively high conductivity in which the charge carrier is a divalent cation. Target systems include MI_2-$M(PO_3)_2$/$M(PS_3)_2$, where 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.

PURDUE UNIVERSITY (continued)

446. INSTRUMENTATION OF X-RAY DIFFRACTION AND MATERIALS RESEARCH ON THE NATIONAL SYNCHROTRON LIGHT SOURCE

G. L. Liedl
School of Materials Engineering
Phone: (317) 494-4095

$445,000 01-1

Development and operation of a high intensity X-ray synchrotron beam line for X-ray diffraction studies involving scientists primarily from midwestern institutions (principal institutions are University of Illinois, Northwestern University, Purdue University, Iowa State University, University of Missouri, and Argonne National Laboratory). Major research efforts on phase transformation studies and X-ray surface diffraction, with specific topics including: substitutional solutes in FCC systems, interstitial solutes, clustering of vacancies in oxides, martensitic transformations non-equilibrium phonons in crystals, phase transitions in 2D systems, structure of small iron particles, structure of organic layers, melting of grain and phase boundaries, electronic materials interfaces, and heterogeneous catalysis.

447. MECHANISMS OF ELEVATED TEMPERATURE RUPTURE IN SINGLE PHASE CERAMICS

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

$91,250 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, UO_2, NiO, carbonyl Ni, and Si_3N_4.

PURDUE UNIVERSITY (continued)

448. 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.

449. 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

$94,308 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."

PURDUE UNIVERSITY (continued)

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

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

$48,300 02-2

A variety of condensed matter science experiments using the unique source of Tungsten-183 with 46.5 keV Mossbauer radiation at the University of Missouri, with intensity about one thousand times more intense than that used in most Mossbauer Spectroscopy experiments. A special Microscopic Conversion Electron (MICE) detector now in service. Experiments to separate the elastic and inelastic scattering at Bragg reflections, to determine the quasielastic linewidths observed in critical phenomena, and to study very low energy Landau excitations will be undertaken.

451. A STUDY OF THE INTERACTION OF LIGHT WITH SUB-MICRON METALLIC SURFACES

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

$100,000 (18 Months) 02-2

Measurements to provide quantitative information about the interaction of laser light in the visible and near ultraviolet with metallic surfaces of sub-micron extent. Studies of the photo-excitation and subsequent emission of electrons at energies below threshold through the surface potential barrier, the thermal effects associated with the illumination of the surface, and the laser-induced diffusion of adsorbates over the sub-micron surface.

RENSSELAER POLYTECHNIC INSTITUTE
Troy, NY 12181

452. TESTS AND MODELING FOR SINTERING THEORY

R. H. Doremus
Dept. of Materials Engineering
Phone: (518) 266-6373
R. M. German
Dept. of Materials Engineering
Phone: (518) 266-6445

$82,000 01-1

Critical assessment of sintering theories. Measurements of particle, grain, and pore size and shape, shrinkage, surface area, and neck size during the sintering of sodium chloride, aluminum oxide, and aluminum-chromium oxide. Measurements and experimental techniques include dilatometry, buoyancy for density, scanning and transmission electron microscopy, X-ray line broadening, mercury porisometry, and BET surface adsoprtion.

453. MECHANISM OF MECHANICAL FATIGUE IN FUSED SILICA

M. Tomozawa
Dept. of Materials Engineering
Phone: (518) 266-6451

$97,000 01-2

Mechanism of static fatigue and analysis of fatigue kinetics in fused silica. Measurement of diffusion coefficient and solubility of water into silica glass as a function of stress, temperature and water vapor pressure. Preparation of silica glass containing various water contents. Effect of water content on swelling and mechanical property alteration. Estimation of mechanical (static) fatigue kinetics by combining stress-accelerated diffusion and swelling data.

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

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

$120,207 02-2

Fundamental problems associated with electrochemical corrosion and catalysis studied through microscopic specification of the structure, energetics, and kinetics of the solid-liquid interface. Novel optical techniques developed and exploited as in situ probes: Raman spectroscopy, modulated reflectivity, ellipsometry, photovoltage spectroscopy, infrared emission, X-ray absorption fine structure, and photon-induced transient relaxation.

RESEARCH INSTITUTE OF COLORADO
Condensed Matter Laboratory
Fort Collins, CO 80526

455. PROPERTIES OF MOLECULAR SOLIDS AT HIGH PRESSURE AND TEMPERATURE

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

$69,861 02-3

Calculations by various techniques of the properties of classes of molecular solids over ranges of temperature and pressure. Properties of interest: equation of state, pressure dependence of lattice vibrational and librational modes, structural and orientational phase transitions, energy transfer mechanisms, virial coefficients, viscosities transport properties, combustion and detonation phenomena and synthesis of new materials.

RICE UNIVERSITY
P. O. Box 1892
Houston, TX 77251

456. 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

$61,058 01-3

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 modelling. Theoretical models based upon Thiele moment expansions and cell cluster techniques for interstitial solid solutions containing secondary defects (e.g., vacancies).

RICE UNIVERSITY (continued)

457. ELECTRON SPIN POLARIZATION EFFECTS IN LEED ION NEUTRALIZATION AND METASTABLE ATOM DEEXCITATION AT SOLID SURFACES

G. K. Walters
Dept. of Physics
Phone: (713) 527-4937
F. B. Dunning
Dept. of Physics
Phone: (713) 527-8101

$200,000 02-2

Polarized Low Energy Electron Diffraction, (PLEED) study of absorption systems: e.g., Ni with Te adsorbed and W with H absorbed. Spin polarization measurements in conjunction with ion neutralization spectroscopy (INS) and metastable deexcitation spectroscopy (MDS) to study surface electronic structure on magnetic materials such as Ni. Polarized He^+ beams used for INS and polarized $He(2^3S)$ beams for MDS.

UNIVERSITY OF ROCHESTER
Rochester, NY 14627

458. FRACTURE TOUGHNESS OF MATERIALS

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

$90,000 01-2

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 using crack-tip shields for the position of dislocations relative to the tips of cracks and thermomechanical measurements of phase transitions in ZrO_2 for phase transformation fracture toughening.

UNIVERSITY OF ROCHESTER (continued)

459. MICROSTRUCTURAL BEHAVIOR OF NON-EQUILIBRIUM SYSTEMS

J. C. M. Li
Dept. of Mechanical Engineering
Phone: (716) 275-4038

$89,975 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.

ROCKWELL INTERNATIONAL SCIENCE CENTER
1049 Camino Dos Rios/Box 1085
Thousand Oaks, CA 91360

460. ADVANCED SILICON NITRIDE SYSTEM STUDIES

F. F. Lange
Phone: (805) 373-4127
P. E. D. Morgan
Phone: (805) 373-4273

$224,924 (9 Months) 01-5

Study of crystal chemistry, phase equilibria, fabrication, and microstructure in the $(ZrO_2/Y_2O_3)/Si_3N_4$ system in an effort to transformation toughen covalent-type ceramics such as Si_3N_4. Use of Si-S chemistry to provide starting points for the preparation of Si_3N_4 and SiC in various forms such as powder, whiskers, fibers, etc. TGA, XRD, TEM, NMR, IR, fracture toughness.

RUTGERS UNIVERSITY
Busch Campus/P. O. Box 909
Piscataway, NJ 08854

461. LOCAL STRUCTURE OF METAL ATOMS IN SILICA AND SILICATES

S. H. Garofalini
Dept. of Ceramics
Phone: (201) 932-2216

$70,980 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.

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

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

$139,500 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.

SETON HALL UNIVERSITY
South Orange, NJ 07079

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

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

$59,817 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.

UNIVERSITY OF SOUTHERN CALIFORNIA
University Park
Los Angeles, CA 90089-1112

464. DEPOSITION, MICROSTRUCTURE, AND PROPERTIES OF LASER CVD FILMS

S. D. Allen
Center for Laser Studies
Phone: (213) 743-6705
S. Copley
Dept. of Materials Science
Phone: (213) 743-6223

$125,081 01-5

Experimental and theoretical research on the laser chemical vapor deposition LCVD process to predict deposition rates, microstructures, and resulting film properties. Effects of surface temperature, laser spot size, local vapor composition, total pressure, optical absorption, thermal properties, and thermal expansion mismatch are isolated in experiments designed to measure chemical, optical, thermal, and mechanical effects. Calculations and measurements of surface temperature and theoretical analysis of convective transport. Model systems to be investigated include LCVD of SiC on SiC substrates, on SiC substrates coated with Mo, and on Mo and W substrates. Film thickness profiles, microstructures, and film adherence are characterized by a variety of techniques.

SOUTHWEST RESEARCH INSTITUTE
6220 Culebra Road
San Antonio, TX 78284

465. 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

$148,000 01-2

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 Al_2O_3 subject to uniaxial tensile stress. Characterization of cavity development and breakaway conditions during the final stage sintering of Al_2O_3. 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: Al_2O_3, SiC.

SRI INTERNATIONAL
Menlo Park, CA 94025

466. MINOR ALLOYING ELEMENTS IN THE PITTING BEHAVIOR OF METALS AND ALLOYS

D. D. Macdonald
Chemistry Laboratory
Phone: (415) 859-3195

$74,825 (6 Months) 01-3

Experimental and theoretical investigation of pitting in austenitic stainless steels (Fe-Ni-Cr-base composition). Extension of the solute/vacancy interaction model to consider breakdown of passive films and role of minor alloying elements thereon, modelling 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.

STANFORD UNIVERSITY
Stanford, CA 94305

467. INTERNAL-VARIABLE BASED MODELS FOR ELEVATED TEMPERATURE FATIGUE AND DEFORMATION

A. K. Miller
Dept. of Materials Science and Engineering
Phone: (415) 497-3732

$190,000 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 modelling work (the development of MATMOD and MATCON constitutive relations) on the plasticity of materials and serves as input to the elevated-temperature fatigue model.

468. MECHANISMS OF HIGH TEMPERATURE CRACK GROWTH IN METALS AND ALLOYS

W. D. Nix
Dept. of Materials Science and Engineering
Phone: (415) 497-4259

$44,471 (5 Months) 01-2

Study of the processes of creep crack extension in simple metals (Cu and Ni), examination of cavitation damage at crack tip 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)

469. ELECTRICAL AND OPTICAL PROPERTIES OF SINGLE CRYSTAL AND THIN FILM II-VI HETEROJUNCTIONS

R. H. Bube
Dept. of Materials Science and Engineering
Phone: (415) 497-2534

$205,000 01-3

Interactions occuring 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 characterzation 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 TEM analysis of heterojunction interfaces, lattice 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.

470. EVALUATION OF MACHINING DAMAGE IN BRITTLE MATERIALS

B. T. Khuri-Yakub
Dept. of Electrical Engineering
Phone: (415) 497-0718

$55,829 (6 Months) 01-5

Investigation of machining damages such as sub-surface slot-like cracks and compressive surface residual stress in brittle materials. Acoustic and laser techniques to measure both the crack sizes and the residual stress. Development of fracture model to predict strength reduction due to machining damage. Slow crack growth effects. Study of Si_3N_4, Si, and SiC.

STANFORD UNIVERSITY (continued)

471. THE USE OF NON-DESTRUCTIVE EVALUATION TECHNIQUES IN THE STUDY OF SMALL FATIGUE CRACKS

Drew V. Nelson
Dept. of Materials Science and Engineering
Phone: (415) 497-2123
John 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.

STEVENS INSTITUTE OF TECHNOLOGY
Hoboken, NJ 07030

472. MAGNETISM IN SOLIDS: SYNCHROTRON RADIATION AND SPIN POLARIZED PHOTOELECTRON STUDIES

G. M. Rothberg
Dept. of Materials and Metallurgical Engineering
Phone: (201) 420-5269

$104,000 02-2

Synchrotron radiation experiments using spin polarized extended X-ray absorption fine structure and the spin dependence of photoelectron diffraction to study the distance and temperature dependencies of spin-spin correlations in bulk magnetic solids and on surfaces. Exploration of the use of energy loss fine structure measurements to complement other techniques for characterization of surfaces.

SYRACUSE UNIVERSITY
Syracuse, NY 13210

473. 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

$104,257 (7 Months) 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 O_2, 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.

UNIVERSITY OF TENNESSEE
Knoxville, TN 37996-1600

474. STATISTICAL MECHANICS OF POLYMER SYSTEMS

J. Kovac
Dept. of Chemistry
Phone: (615) 974-3444

$86,000 03-1

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 themodynamics, 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.

UNIVERSITY OF TEXAS
Austin, TX 78712

475. THE NATURE OF PHOTOEMISSION IN DIELECTRIC FLUIDS

J. C. Thompson
Dept. of Physics
Phone: (512) 471-5926
P. R. Antoniewicz
Dept. of Physics
Phone: (512) 471-3766

$27,000 (8 Months) 02-2

Studies of photoemission from electrodes into dielectric fluids and time of charge transport by pulse injection techniques as function of photon energy, potential, and temperature. Experimental studies: surface roughness, adsorbates, double layer structure, scavengers, solvent structure, laser intensity, and time evolution of charge injection. Density of states calculations and development of models for photo-injection into dielectric media.

UNIVERSITY OF UTAH
Salt Lake City, UT 84112

476. 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, 3589, 6863

$83,000 01-1

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)

477. FABRICATION, PHASE TRANSFORMATION STUDIES AND CHARACTERIZATION OF SIC-ALN-AL(2)OC CERAMICS

A. V. Virkar
Dept. of Materials Science and Engineering
Phone: (801) 581-5396

$96,000 01-1

Preparation of SiC-AlN-Al_2OC powders by a carbothermal reaction of a mixture of SiO_2 and Al_2O_3 in N_2 or argon. Fabrication of SiC-AlN-Al_2OC ceramics by hot pressing, and subjecting such dense, hot pressed ceramics to various annealing treatments. X-ray diffraction and STEM analysis to investigate phase equlibria, 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.

478. THEORETICAL AND EXPERIMENTAL STUDY OF SOLID PHASE MISCIBILITY GAPS IN III/V ALLOYS

G. B. Stringfellow
Dept. of Materials Science and Engineering
Phone: (801) 581-8387

$87,198 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 $GaAs_{0.5}Sb_{0.5}$ alloys on hole and electron mobility and photoluminescence half-widths. Raman spectroscopy and STEM analysis of spinodal compositions and clustering.

UNIVERSITY OF VIRGINIA
Charlottesville, VA 22901

479. 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

$76,995 01-2

Experimental correlation of fatigue behavior of duplex martensitic-ferritic steels, determination of relationship between continuous hard and soft phases (martensite and ferrite) and effects of carbide structure, distribution and morphology as studied by TEM. Control of microstructure by thermomechanical processing of Fe-C-Mn, Fe-C-Mo, Fe-C-V and Fe-C-Mn-V alloys. Correlative studies involving cyclic stress strain response, hardening, softening, microstructure stability under cyclic loading, damage accumulation, crack initiation and propagation in high and low cycle fatigue, micromechanisms, crack closure effects.

480. SPECTROSCOPY OF SURFACE ADSORBED MOLECULES

R. V. Coleman
Dept. of Physics
Phone: (804) 924-3781

$111,889 02-2

Elastic and inelastic tunneling characteristics of junctions doped with inorganic and organic molecules. Modifications of the tunnel barrier heights due to surface and interface interactions and charge transfer analyzed using computer model fits to experimental I versus V curves. Electric field induced modifications of barrier heights due to metastable electronic states are being detected due to doping with organic molecules having high π-resonance energy and to Si and C dopants. Chemical shift data from photoelectron spectroscopy (ESCA) for correlation with tunneling results. Tunneling experiments leading to the development of an electron tunneling microscope are also underway.

UNIVERSITY OF VIRGINIA (continued)

481. MAGNETIC IMPURITIES IN SUPERCONDUCTORS

J. Ruvalds
Dept. of Physics
Phone: (804) 924-3782

$97,000 02-3

Theoretical research on the influence of magnetic impurity interactions in superconductors on the upper critical magnetic field, H_{c2}. Investigation of rare earth impurities in various metallic hosts to determine relative importance of exchange interactions and of electronic structural basis for coupling. Studies on influence of dilute and moderate concentrations of impurities on the electron spin susceptibility, resistivity, and nuclear spin relaxation rate. Emphasis on new mechanisms for achieving enhancement of superconducting properties in high magnetic fields. Properties of heavy fermion superconductors and the motion of charge density and spin density waves in electromagnetic fields.

WASHINGTON UNIVERSITY
St. Louis, MO 63130

482. NON-EMPIRICAL INTERATOMIC POTENTIALS FOR TRANSITION METALS

A. E. Carlsson
Dept. of Physics
Phone: (314) 889-5739

$55,000 (16 Months) 02-3

Development of existing scheme for calculating interatomic potentials in simplified tight-binding models into a method applicable to transition metals. 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.

UNIVERSITY OF WASHINGTON
Seattle, WA 98195

483. 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.

484. FUNDAMENTAL STUDIES OF ELASTOMERS

B. E. Eichinger
Dept. of Chemistry
Phone: (206) 543-5900

$101,935 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, viscoeleastic 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.

UNIVERSITY OF WEST VIRGINIA
Morgantown, WV 26506

485. ELECTRON HYBRIDIZATION EFFECTS AND THE CRYSTAL STRUCTURE OF PLUTONIUM

B. R. Cooper
Dept. of Physics
Phone: (304) 293-3423

$58,401 03-1

Investigation of the crystalline allotropic peculiarities of elemental plutonium with detailed calculations of the electronic structure, including correlation effects and the pertinent contributions to the lattice energy. This work will be based on a theoretical framework of electron hybridization effects. Insight into the bonding behavior of Pu will also be obtained by developing a theory of the PuTe(x)Sb(1-x) system in conjunction with planned experiments.

UNIVERSITY OF WISCONSIN
Madison, WI 53706

486. 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.

UNIVERSITY OF WISCONSIN (continued)

487. 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^{R} 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.

488. 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

$86,260 01-1

Experimental investigation of the structure, stability, and atomic transport behavior of high-T_g 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 inter-diffusion 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.

UNIVERSITY OF WISCONSIN (continued)

489. OPTICAL STUDIES OF DYNAMICAL PROCESSES IN DISORDERED MATERIALS

W. M. Yen
Dept. of Physics
Phone: (608) 263-7475

$95,000 02-2

A comprehensive study of relaxation and energy transfer properties of impurity-activated disordered systems and exploratory investigations of doped ceramics. A capability to measure coherent optical transient effects developed for use in conjunction with an existing facility for fluorescence line narrowing. Investigation of the temperature dependence of the relaxation effects in disordered materials and testing of disordered materials to determine the microscopic interactions and to extend models. Fundamental study of ion transfer, trapping, and cross relaxation in prototypical luminescent glass systems.

490. SURFACE EXCITATIONS AND THEIR INTERACTION WITH LOW ENERGY ELECTRONS

S. Y. Tong
Dept. of Physics and Surface Studies Laboratory
Phone: (414) 963-4474

$88,000 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 with D. L. 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.

ADELPHI TECHNOLOGY
13800 Skyline Blvd.
Woodside, CA 94062

501. THE CONSTRUCTION OF A SOFT X-RAY SOURCE USING TRANSITION RADIATION FOR LITHOGRAPHY

M. A. Piestrup
President
Phone: (415) 851-0633

$49,928 (6 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 curent for maximum flux and target lifetime.

ANALYSIS CONSULTANTS
21831 Zuni Drive
El Toro, CA 92630

502. THE DESIGN AND FABRICATION OF FLAT PANELS WITH HIGH ACOUSTIC TRANSMISSIVITY

B. G. Martin
President
Phone: (714) 380-1204

$38,500 (6 Months) SBIR

Feasiblity 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.

THE ARIZONA CARBON FOIL COMPANY INC.
4152 E. Sixth Street
Tucson, AZ 85711

503. THICK HARD CARBON COATINGS FOR PROTECTION OF MECHANICAL AND OPTICAL COMPONENTS

J. O. Stoner
Vice President
Phone: (602) 621-6814

$49,925 (6 Months) SBIR

Production of stress-free carbon coatings thicker than two micrometers using an rf powered coater. Identification of optimum coating parmeters for low-stress coatings on optical glass, silicon, and germanium surfaces. Coatings will be tested for mechanical and chemical resistance.

CERAMATEC INC.
163 West 1700 South
Salt Lake City, UT 84115

504. FABRICATION AND CHARACTERIZATION OF CERAMIC MATRIX-CERAMIC WHISKER COMPOSITES WITH RANDOM ORIENTATION OF THE WHISKERS

L. Viswanathan
Senior Research Scientist
Phone: (801) 486-5071

$49,884 (6 Months) SBIR

Fabrication and charcterization of ceramic matrix-SiC whisker composites by pressureless sintering for advanced heat engines. Development of powder processing methods that yield randomly oriented whiskers. The materials to be studied are Al_2O_3 + SiC and Si-Al_2OC + 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.

MATERIALS & ELECTROCHEMICAL RESEARCH CORP.
4660 N. Via Madre
Tucson, AZ 85749

505. THE DIRECT PRODUCTION OF INTERMETALLIC COMPOUND POWDER

J. C. Withers
Technical Manager
Phone: (602) 749-3257

$50,000 (6 Months) SBIR

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 Ni_3Al 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.

SPIRE CORPORATION
Patriots Park
Bedford, MA 01730

506. SELF-LUBRICATING DIAMOND-LIKE COATING BY A SIMULTANEOUS SPUTTER-DEPOSITION/ION-IMPLANTATION PROCESS

P. Sioshansi
Vice President, Surface Modification Center
Phone: (617) 275-6000

$49,991 (6 Months) SBIR

Development of a simultaneous sputter-coating, ion-implantation technique for creation of diamond-like thin films with excellent adhesion and parameters close to those of the bulk material. Coatings studied are carbon and boron nitride.

TECHNICAL RESEARCH ASSOCIATES INC.
410 Chipeta Way
Salt Lake City, UT 84108

507. CASTABLE GOLD CERMET FOR ELECTRICAL CONTACTS

C. D. Baker
Vice President
Phone: (801) 582-8080

$50,000 (6 Months) SBIR

Production of low-denstiy, oxide-dispersion-strengthened gold-silica cermet. The cermet will consist of gold (70% by volume), with fully-wetted, fine dispersed silica particles. The objective is to produce a castable and recastable material that retains the desirable physical properties of bulk gold such as corrosion protection and low electrical contact resistance, but with improved properties such as hardness and cold flow.

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.

AMERICAN RESEARCH CORPORATION OF VIRGINIA
642 First St., P.O. Box 3406
Radford, VA 24143-3406

508. EDDY CURRENT NONDESTRUCTIVE EVALUATION OF LASER GLAZED METALLIC SURFACES

R. J. Churchill
President
Phone: (703) 639-9542

$245,112 SBIR

Eddy current nondestructinve evaluation techniques to characterize melt depth and to detect flaws in laser glazed metallic surfaces. Principal Phase I findings include a correlation between blaze 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.

CERAMATEC INC.
163 West 1700 South
Salt Lake City, UT 84115

509. PROCESSING AND CHARACTERIZATION OF SICALON CERAMICS

Raymond A. Cutler
Program Manager
Phone: (801) 486-5071

$249,563 SBIR

Liquid phase sintering of SiCAlON 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 Al2OC content to demonstrate the ceramic engineering possible with SiCAl2OC. Novel sintering techniques to show economical desification of SiAlON ceramics. Elevated temperature strength and creep measurements to determine the temperature range where liquid phase sintered SiCAlON can be applied. Investigation of the stability of the solid solution in air, N2, and Ar at temperatures up to 1700 ^{o}C.

CERAMIC FINISHING COMPANY
P. O. Box 498
State College, PA 16804

510. FRACTURE MECHANICS INVESTIGATION OF GRINDING OF CERAMICS

Henry P. Kirchner
President
Phone: (814) 238-4270

$107,988 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.

CERES CORPORATION INC.
202 Boston Road
North Billerica, MA 01862

511. 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.

ELECTROCHEMICAL TECHNOLOGY CORPORATION
3935 Leary Way, N.W.
Seattle, WA 98107

512. MATHEMATICAL MODELING OF ELECTROCHEMISTRY OF STRESS CORROSION CRACKING

T. R. Beck
Phone: (206) 632-5965

$167,586 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.

KJS ASSOCIATES
1616 Hillrose Place
Fairborn, OH 45342

513. DEVELOPMENT OF ND-FE-B METAL-MATRIX MAGNETS

Reinhold M. W. Strnat
Research Engineer
Phone: (513) 299-0313, 2717

$113,466 SBIR

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 constiturent after aging.

SUPERCON INC.
9 Eric Drive
Natick, MA 01760

514. 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 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.

UNIVERSAL ENERGY SYSTEMS INC.
4401 Dayton-Xenia Road
Dayton, OH 45432

515. FABRICATION OF AMORPHOUS METALLIC FILMS AND COATINGS FOR INDUSTRIAL APPLICATION USING HIGH ENERGY ION BEAM MIXING

Peter P. Pronko
Chief Scientist
Phone: (513) 426-6900

$245,212 SBIR

Fabrication of amorphous Ni- and Cu-base metallic films and coatings using deeply penetrating high energy ion beam mixing. Use of the so-called structural difference rule for amorphous alloy formation by ion mixing. Evaluation of modified surfaces in erosive and corrosive pitting conditions, e.g., involving exposure to electro-hydrodynamic and corrosive fluid dynamic environments and comparison with crystalline metal behavior.

SECTION D

"Major User Facilities"
(Large Capital Investment)

NATIONAL SYNCHROTRON LIGHT SOURCE

Brookhaven National Laboratory
Upton, New York 11973

The National Synchrotron Light Source (NSLS) 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 the synchrotron radiation include high brightness and intensity, its broad and continuous spectral range, high polarization and pulsed time structure (subnanosecond pulses). With each of the 28 X-ray and 16 VUV beam ports being further split into from 2 to 4 beam lines, it will be possible to have as many as 100 experiments running 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 presently being designed which will significantly increase the photon intensity and brightness.

The NSLS is a facility where a wide range of research techniques are being utilized 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 experimental utilization 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 in the process of forming insertion device teams (IDTs) to design and instrument beam lines and insertion devices.

General Users are able to perform experiments on an NSLS facility beam line or on a PRT beam line which 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. After an initial commissioning period, NSLS and PRT beam lines become available for use by General Users.

Proprietary research can be performed at the NSLS. A full-cost recovery fee will be charged for the amount of beam time utilized. 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.

A limited amount of funding is available to scientist 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 reserach, 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
Upton, NY 11973

NATIONAL SYNCHROTRON LIGHT SOURCE

TECHNICAL DATA

Facilities	Key Features	Operating Characteristics
VUV electron storage ring	high brightness, continuous wavelength range ($\lambda > 5$ Å) 16 beam ports.	0.75 GeV electron energy
X-ray electron storage ring	high brightness, continuous wavelength range ($\lambda > .5$ Å) 28 beam ports	2.5 GeV electron energy

Instruments

Monochromators:

plane grating	12 Å $< \lambda <$ 1500 Å; high resolution
zone plate	8 Å $< \lambda <$ 100 Å; moderate resolution
toroidal grating	10 Å $< \lambda <$ 2500 Å; high intensity, moderate and high resolution
extended range grasshopper	10 Å $< \lambda <$ 2000 Å; high resolution
Wadsworth	300 Å $< \lambda <$ 3000 Å; high intensity, moderate resolution
Seya&Czerny Turner	1200 Å $< \lambda <$ 12000 Å; high intensity, moderate resolution
two crystal	.04 Å $< \lambda <$ 2500 Å; high resolution, fixed exit beam
two crystal/two grating	2.5 Å $< \lambda <$ 2500 Å; 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 Å $< \lambda <$ 5000 Å; high intensity and brightness

HIGH FLUX BEAM REACTOR

Brookhaven National Laboratory
Upton, New York 11973

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 = 1.0×10^{15} neutrons/cm^2-sec). The HFBR was designed to provide particularly pure beams of thermal neutrons, uncontaminated by fast neutrons and by gamma rays. A cold source (liquid hydrogen moderator) provides enhanced flux at long wavelengths ($\lambda > 4$ A). A polarized beam spectrometer, triple-axis spectrometers and small-angle scattering facilities are among the available instruments. Special equipment for experiments at high and low temperatures, high magnetic fields, and high pressure are 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 merity 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
HFBR - Bldg. 750
Brookhaven National Laboratory
Upton, New York 11973

(516) 282-4056
FTS 666-4056

HIGH FLUX BEAM REACTOR

TECHNICAL DATA

Instruments	Purpose and Description
Solid State Physics	
4 Triple-axis Spectrometers	Inelastic scattering; diffuse scattering; powder diffractometer; polarized beam. Energy range: 2.5 meV $< E_o <$ 200 meV Q range: $0.03 < Q < 10$ Å^{-1}
Biology	
Small Angle Neutron Scattering	Studies of large molecules. Located on cold source with 20 x 20 cm^2 position-sensitive area detector. Sample detector distance L < 2 meter Incident wavelength 4 Å $< \lambda_o <$ 10 Å
Diffractometer	Protein crystallography 20 x 20 cm^2 area detector λ_o = 1.57 Å
Chemistry	
2 Diffractometers	Single-crystal elastic scattering 4-circle goniometer 1.69 Å $< \lambda_o <$ 0.65 Å
1 Triple-axis Spectrometer	Inelastic scattering Diffuse scattering Powder diffractometry
Nuclear Physics	
3 Spectrometers	Neutron capture studies Energy range: 0.025eV $< E_o <$ 25keV
TRISTAN II (Isotope Separator)	Spectroscopic study of neutron-rich unstable isotopes produced from U-235 fission
Irradiation Facilities	
7 Vertical Thimbles	Neutron activation; production of isotopes; thermal flux: 8.3×10^{14} neutrons/cm^2 sec; fast (> 0.5 MeV) flux: 3×10^{14} neutrons/cm^2 sec.

NEUTRON SCATTERING AT THE HIGH FLUX ISOTOPE REACTOR

Solid State and Chemistry Divisions
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

The neutron scattering facilities at the High Flux Isotope Reactor (HFIR) are used for long-range basic research on the structure and dynamics of condensed matter. Active programs exist on the magnetic properties of matter, lattice dynamics, defect-phonon interactions, 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 5×10^{15} neutrons/cm^2 s, and the flux at the inner end of the beam tubes is slightly greater than 10^{15} neutrons/cm^2 s. 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

H. A. Mook
Solid State Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

(615) 574-5242
FTS 624-5242

NEUTRON SCATTERING AT THE HIGH FLUX ISOTOPE REACTOR

Technical Data

Beam No.	Instrument	Operating Characteristics
HB-1	Triple-axis polarized-beam	Beam size - 2.5 by 3 cm max Flux - 2.6 x 10^6 neut/cm^2 s at sample (polarized) Vertical magnetic fields to 5 T Horizontal fields to 2 T Variable E_o
HB-1A	Triple-axis, fixed E_o	E_o = 14.7 MeV, 2.353 angstroms Beam size - 5 by 3.7 cm max Flux - 9 x 10^6 neut/cm^2 s at sample with 40 ft collimation
HB-2A	Liquid diffractometer with linear position sensitive detector	Beam size - 1 by 3.4 cm max Wavelength = 0.89 angstrom Flux - 6.8 x 10^5 neut/cm^2 s at sample with 20 ft collimation
HB-2, HB-3	Triple-axis, variable E_o	Beam size - 5 by 3.7 cm max Flux - 10^7 neut/cm^2 s at sample with 40 ft collimation
HB-3A	Double-crystal small-angle diffractometer	Beam size - 4 x 2 cm max Flux - 10^4 neut/cm^2 s Wavelength - 2.6 angstroms Resolution - 4 x 10^{-5} angstroms^{-1}
HB-4A	Four-circle diffractometer	Beam size - 5 x 5 mm Flux - 2 x 10^6 neut/cm^2 s with 9 ft collimation Wavelength = 1.015 angstrom
	Wide-angle time-slicing diffractometer	Beam size - 2 x 3.7 cm max Flux - 2 x 10^6 neut/cm^2 s with 9 ft collimation Wavelength=1.015 angstrom Curved linear position sensitive detector covering 130°
HB-4	Correlation chopper	Beam size - 5 x 3.7 cm Flight path - 1.5 m 70 detectors covering 130° Variable E_o Variable pulse width

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 x 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

G. H. Lander, Program Director	(312) 972-5518 FTS 972-5518
B. S. Brown, Operations Manager	(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

IPNS EXPERIMENTAL FACILITIES

NEUTRON SCATTERING

Facility (Instrument Scientist)	Assignment	Range †Wave-vector	Range Energy	Resolution Wave-vector	Resolution Energy
Special Environment Powder Diffractometer (J. D. Jorgensen)	F5	0.5-50 $Å^{-1}$	*	0.35%	*
General Purpose Powder Diffractometer (J. Faber, Jr.)	F2	0.5-100 $Å^{-1}$	*	0.25%	*
Single Crystal Diffractometer (A. J. Schultz)	H1	2-20 $Å^{-1}$	*	2%	*
Low-Resolution Medium-Energy Chopper Spectrometer (C.-K. Loong)	F4	0.1-30 $Å^{-1}$	0-0.6 ev	0.02 k_o	0.05 E_o
High-Resolution Medium-Energy Chopper Spectrometer (D. L. Price)	H3	0.3-9 $Å^{-1}$	0.-0.4 eV	0.01 K_o	0.02 E_o
Small-Angle Scattering Diffractometer (J. E. Epperson)	C1	0.008-0.3 $Å^{-1}$	*	0.004 $Å^{-1}$	*
Crystal Analyzer Spectrometer (T. O. Brun)	F1	3-16 $Å^{-1}$	0.02-0.5 eV	3%	2%

* No energy analysis
† Wave-vector, $K = 4\pi \sin \theta/\lambda$

NEUTRON BEAMS FOR SPECIAL EXPERIMENTS

Beam Tube	Current Use	Flight Path Length (m)
F3	eV Spectrometer	10
C2	Polarized Neutron Exp.	10
C3	Solid He^3 Project	10
F6	Irradiations	6-20
H2	Irradiations	6-20
V1	Ultra-Cold Neutron Exp.	4

LOS ALAMOS NEUTRON SCATTERING CENTER

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

The Los Alamos Neutron Scattering Center (LANSCE) facility is a pulsed spallation neutron source driven by the 800-MeV Los Alamos Meson Physics (LAMPF) linear accelerator. Neutron scattering research is currently carried out at LANSCE using the advantages of time-of-flight methods and high epithermal flux. Available instruments are: a) 32 m neutron powder diffractometer; b) a single crystal diffractometer based on the Laue-TOF technique; c) a filter difference spectrometer for chemical and optic mode spectroscopy; d) a constant-Q spectrometer for studies of elementary excitations in single crystals, and e) a liquids, amorphous, and special environment diffractometer. A considerable effort is directed toward pulsed source instrument development including, currently, a chopper spectrometer and a low Q diffractometer. A proton storage ring (PSR) has begun operation in 1985, which will provide at 12 neutron bursts per second the world's highest peak thermal flux for neutron scattering research. In addition, it will also be a source of epithermal neutrons many orders of magnitude larger than reactors for neutron scattering research in solid state physics, chemistry, biology, polymers, 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 R. Silver 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 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 LANSE 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 non-sensitive countries. DOE approval is required for any other foreign national visits.

PERSON TO CONTACT FOR INFORMATION

R. N. Silver
MS H805, Group P-8
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

(505) 667-6069 or
(FTS) 843-6069

LANSCE

TECHNICAL DATA

	1984	1985
Proton Source	LAMPF	LAMPF + PSR
Proton Source Current	1000μA	1000μA
Proton Source Energy	800MeV	800MeV
SNR Proton Current	3.5μA	100μA
Proton Pulse Width	5μs	0.27μs
Repetition Rate	120Hz	12Hz
Epithermal Neutron Current (n/eV.Sr.S)	$1.1 \times 10^{11}/E$	$3.2 \times 10^{12}/E$
Peak Thermal Flux ($n/cm^2.S$)	6×10^{13}	1.7×10^{16}

Instruments

32 m Neutron Powder Diffractometer (J. Goldstone, Responsible)	Powder diffraction Wave vector 0.3-50A^{-1} Resolution 0.15%
Single Crystal Diffractometer (P. Vergamini, G. Christoph, Responsible)	Laue time-of-flight spectrometer Wave vector 1-15A^{-1} Resolution 2% typical
Filter Difference Spectrometer (J. Eckert, Responsible)	Inelastic neutron scattering, vibrational spectroscopy Energy trans. 25-600 meV Resolution 5-7%
Liquids, Amorphous & Special Environment Diffractometer (A. Williams, Responsible)	Low resolution (.7%) powder, and liquids and amorphous diffraction at low angles at 2% resolution
Constant-Q Spectrometer (R. Robinson, Responsible)	Elementary excitations in single crystal samples Resolution 1-3%

STANFORD SYNCHROTRON RADIATION LABORATORY

Stanford University
Stanford, California 94305

SSRL is a National Users' Research Laboratory for the application of synchrotron radiation to research in biology, chemistry, engineering, materials science, medicine and physics. SSRL is also developing specialized techniques and instrumentation for the generation and experimental utilization of synchrotron radiation. SSRL presently has 19 experimental stations. The radiation on eight stations is enhanced by insertion devices providing the world's most intense X-ray sources, and brightest soft X-ray source.

A new beam line is under construction on the 16 GeV storage ring, PEP. When completed in the fall of 1985 it will provide an order of magnitude increase in the X-ray spectral brilliance over SSRL's presently brightest lines.

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. Accelerator physics and insertion device development for the production of synchrotron radiation.

SSRL serves approximately 500 scientists from 124 institutions working on over 200 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 60 percent 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

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.

	Horizontal Angular Acceptance (Mrad)	Mirror CutOff (KeV)	Monochromator	Energy Range (eV)	Resolution ΔE/E	Approximate Spot Size HgtxWdth (mm)	Dedicated Instrumenation
INSERTION DEVICE STATIONS							
WIGGLER LINES - X-RAY							
End Stations							
IV-2 (8 pole)							
Focused	3.0	10.2	Double Crystal	2800-21000	$\sim 5\times10^{-4}$	2.0 x 6.0	
Unfocused	1.0	-	Double Crystal	2800-45000	$\sim 10^{-4}$	2.0 x 20.0	
VI-2 (54 pole)							
Focused	3.0	22	Double Crystal	2800-21000	$\sim 5\times10^{-4}$	2.0 x 6.0	
Unfocused	1.0	-	Double Crystal	2800-45000	$\sim 10^{-4}$	2.0 x 20.0	
VII-2 (8 pole)							Six-circle Diffractometer
Focused	3.0	10.2	Double Crystal	2800-4500	$\sim 5\times10^{-4}$	2.0 x 6.0	
Unfocused	1.0	-	Double Crystal	2800-21000	$\sim 10^{-4}$	2.0 x 20.0	
Side Stations							
IV-1	1.0	-	Double Crystal	2800-45000	$\sim 5\times10^{-4}$	2.0 x 20.0	
IV-3	1.0	-	Double Crystal	2800-45000	$\sim 10^{-4}$	2.0 x 20.0	Two-circle Diffractometer
VII-1	1.0	-	Curved Crystal	6000-13000	$\sim 8\times10^{-4}$	0.6 x 3.0	Rotation Camera
VII-3	1.0	-	Double Crystal	2800-45000	$\sim 10^{-4}$	2.0 x 20.0	
UNDULATOR LINES - VUV/SOFT X-RAY							
V-1	1.5	-	None	10-1200	≥7%	6.0 x 8.0	Variable Apertures
UNDULATOR LINES - X-RAY							
PEP	Full	15.0	Double Crystal	120000-20000	$\sim 10^{-4}$	0.6 x 6.0	
BENDING MAGNET LINES							
X-RAY							
I-4	2.2		Curved Crystal	6000-9500	~ 60 eV	0.25 x 0.5	
I-5	1.0	-	Double Crystal	3800-29300	$\sim 10^{-4}$	2.0 x 20.0	Area Detector/CAD-4
II-2 (focused)	4.8	8.9	Double Crystal	2800-8900	$\sim 5\times10^{-4}$	2.0 x 4.0	
II-3	1.0	-	Double Crystal	2800-30000	$\sim 5\times10^{-4}$	2.0 x 20.0	
II-4	1.0	-	None	3200-30000		4.0 x 15.0	
Lifetimes Port	1.8	-	None	1-6	Bandpass >10A	4.0 x .4	
VUV/SOFT X-RAY							
I-1	2.0		Grasshopper	32-1000	Δλ = .1-.2A	2.0 x 1.0	
I-2	4.0		Seya-Namioka	4-40	Δλ = .2-6A	1.0 x 3.0	
III-1	2.0		Grasshopper	15-1200	Δλ = .05-2A	1.0 x 1.0	
III-3	8-10		Jumbo	800-4000	0.35-7 eV	2.0 x 4.0	
III-4	2.0		Multilayer	2-3000	White or $\Delta\lambda/\lambda$=.3%	2.0 x 11	Vacuum Diffractometer/ Exposure Station

Specialized Portable Beam Line Instrumentation Available: VG Chamber, Perkin Elmer Chamber, CAD-4, SAS Camera

SECTION E

"Other User Facilities"

NATIONAL CENTER FOR SMALL-ANGLE SCATTERING RESEARCH

Solid State Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

The National Center for Small-Angle Scattering Research 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

W. C. Koehler, Director NCSASR
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831
(615) 574-5232
FTS 624-5232

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Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831
(615) 574-5237
FTS 624-5237

J. S. Lin, SAXS-NCSASR
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831
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Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831
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M. Gillespie, Secretary NCSASR
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831
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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: 10^4-10^6 neutrons/cm^2 s depending on slit sizes and wavelength

10-m SAXS Instrument Specifications

Monochromator: hot-pressed pyrolytic graphite
Incident wavelengths: 1.542 angstoms (CuK_{alpha}) or 0.707 angstoms (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: $3 \times 10^{-3} \leq K \leq 0.3$ angstoms^{-1} (CuK_{alpha})
$6 \times 10^{-3} \leq K \leq 0.6$ angstoms^{-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

ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH

Argonne National Laboratory
Argonne, Illinois 60439

The Argonne National Laboratory Electron Microscopy Center for Materials Research provides unique facilities which combine the techniques of high-voltage electron microscopy, ion-beam modification, and ion-beam analysis, along with analytical electron microscopy.

The cornerstone of the Center is a High Voltage Electron Microscope (an improved Kratos/AEI EM7) with a maximum voltage of 1.2 MV. This HVEM is interfaced to two accelerators, a National Electrostics 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). 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 FTS 972-5222
H. Wiedersich (312) 972-5079
Electron Microscopy Center for Materials Research FTS 972-5079
Materials Science and Technology Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH

TECHNICAL DATA

Electron Microscopes	Key Features
High-Voltage Electron Microscope Kratos/AEI EM7 (1.2 MeV)	Resolution 3.5 Å lattice Continuous voltage selection (100-1200 kv) Current density 15 A/cm^2 High-vacuum specimen chamber Negative-ion trap Electron and ion dosimetry systems Video recording system Ion-beam interface Specimen stages 10 - 1300 K Straining and environmental stages
Transmission Electron Microscope Philips EM 420 (120 keV)	Resolution 2.0 Å lattice Equipped with EELS, XEDS Specimen stages 15 - 300 K
Transmission Electron Microscope JEOL 100 CX (100 keV)	Resolution 2.0 Å lattice Equipped with STEM, XEDS Specimen stages 300 - 900 K
Analytical Electron Microscope Being acquired (300 keV)	State-of-the-art resolution Ultra-high vacuum, Field Emission Gun Equipped with EELS, XEDS, etc.
Accelerators	
NEC Model 2 UDHS	Terminal voltage 2 MV Energy stability $\pm$250 eV Current density: H^+, 10 μA/cm^2 (typical) Ni^+, 3 μA/cm^2
Texas Nuclear 300-kV	Terminal voltage 300 kV Energy stability $\pm$300 eV Current density: He^+, 200 μA/cm^2 (typical) Ni^+, 2 μA/cm^2
NEC 600 kV Injector Being acquired	Terminal voltage 600 kV Energy stability $\pm$60 eV Current density: He^+, 100 μA/cm^2 (typical) Ar^+, 10 μA/cm^2

SHARED RESEARCH EQUIPMENT PROGRAM (SHaRE)

Metals and Ceramics Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

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 analytical transmission 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.

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. Curent members are Drs. E. A. Kenik, Chairman, P. S. Sklad, C. B. Carter, 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

E. A. Kenik
Metals and Ceramics Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831
(615) 574-5066
FTS 624-5066

A. Wohlpart
Oak Ridge Associated Universities
P. O. Box 117
Oak Ridge, Tennessee 37831
(615) 576-3422
FTS 626-3422

SHARED RESEARCH EQUIPMENT PROGRAM (SHaRE)

Technical Data

Instruments and Facilities	Key Features	Operating Characteristics
Hitachi HU-1000 High Voltage Electron Microscope	Heating stages; in situ deformation stages; low light level videorecording system; environmental cell - 0-1 atm	0.3-1.0 MeV; in situ studies electron irradiation studies; ten 4-h shifts/week; available evenings, weekends to qualified users
Philips EM400T/ FEG Analytical Electron Microscope	TEM resolution ~0.2 nm; STEM resolution ~1.0 nm; EDS, EELS, CBEB	120 kV; ten 4-h shifts/week; available evenings, weekends, to qualified users; structural and elemental microanalysis; minimum probe diameter ~1 nm
JEM 120CX Analytical Electron Microscope	TEM resolution ~0.34 nm STEM resolution ~3 nm EDS, EELS, CBED	120 kV; ten 4-h shifts/week; structural and elemental microanalysis; minimum probe diameter <10 nm
JEM 120C Transmission Electron Microscope	TEM resolution ~0.34 nm; special polepiece for TEM of ferromagnetic materials	120 kV; ten 4-h shifts/week; structural microanalysis
PHI 590 Scanning Auger Electron Spectroscopy System	200 nm beam size; fracture stage; residual gas analysis; sputter depth profiling; elemental mapping	Surface analytical and segregation studies
Varian Scanning Auger Electron Spectroscopy System	5 micrometer beam size; hot-cold fracture stage; residual gas analysis; sputter depth profiling; elemental mapping	Surface analytical and segregation studies; gas-solid interaction studies
Dual Ion-Beam Accelerator Facilities	4 MV Van de Graaff accelerator; 400 kV accelerator; sputter depth profiling	Nuclear microanalysis; Rutherford backscattering; elemental analysis
Philips EM430T Analytical Electron Microscope	300 kV, STEM, EDS, EELS; TEM resolution <0.2 nm	300 kV, ten 4 h shifts/week; available evenings, weekends to qualified users; structural and elemental microanalysis
Atom Probe/ Imaging Atom	Atomic resolution imaging; single atom analysis;	To be delivered FY 1985

CENTER FOR MICROANALYSIS OF MATERIALS

Materials Research Laboratory
University of Illinois
Urbana-Champaign, Illinois 61801

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 (217)-333-8396
Center for Microanalysis of Materials
Materials Research Laboratory
University of Illinois
104 S. Goodwin
Urbana, Illinois 61801

CENTER FOR MICROANALYSIS OF MATERIALS

Instruments	Features and Characteristics
Imaging Secondary Ion Microprobe Cameca IMS 3f	Dual ion sources (C_s^+,O_2^+). Depth profiling and mass analyzed secondary ion images with 1 μm resolution.
Scanning Auger Microprobe Physical Electronics 595	Resolution: SEM 30 nm, Auger 70 nm. Windowless X-ray detector.
Scanning Auger Microprobe Physical Electronics 545	Resolution: SEM 3μm.
XPS Physical Electronics 548	Double pass CMA. ESCA and Auger. Specimen temp. to 1550K
Transmission Electron Microscope Philips EM430 (300kV)	EDS, EELS, STEM
Transmission Electron Microscope Philips EM420 (120kV)	EDS (Windowless), EELS, STEM, Cathodoluminescence Cold stage (30K). Computer Control.
Transmission Electron Microscope Philips EM400T (120kV)	EDS. Heating, cooling stages.
Scanning Transmission Electron Microscope Vacuum Generators HB5 (100kV)	0.5 nm probe, field emission gun, EDS, EELS.
Scanning Electron Microscope JEOL JSM 35C (35kV)	5 nm resolution, EDX, channelling and backscattering patterns.
Rutherford Backscattering (in-house construction) (3 MeV)	Two work stations, channelling
X-ray Equipment Elliott 14 kW high brilliance source Rigaku 12 kW source Several conventional sources	4-circle diffactometer. Small angle camera. EXAFS. Lang topography. Powder cameras, etc.

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.

SURFACE MODIFICATION AND CHARACTERIZATION COLLABORATIVE RESEARCH CENTER

Solid State Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

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. Because of the tremendous interests expressed in these techniques and the broad range of existing collaborations, plans for a users' facility have been initiated. Until this program has been established, the informal arrangement will be continued. 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

SURFACE MODIFICATION AND CHARACTERIZATION COLLABORATIVE RESEARCH CENTER

Technical Data

Accelerators	Operating Characteristics
2.5-MV positive ion Van de Graaff	0.1-3.2 MeV; H, D, ^{4}He, ^{3}He, and selected gases. Beam current ~50 microamps
1.7-MV tandem	0.2-3.5 MeV H; 0.2-5.1 MeV ^{3}He, ^{4}He; negative ion sputtering source for heavy ion beams of most species to 7 MeV
10-200-KV high-current ion Implantation Accelerator	Essentially any species of ion; 1-3 mamps singly charged, ~100 microamps doubly and triply charged
0.1-10-KeV Ion Gun	Gaseous species; ~20 microamps
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; laser fluorescence spectroscopy; 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

COMBUSTION RESEARCH FACILITY - MATERIALS PROGRAM

Sandia National Laboratories
Livermore, California 94550

Optical techniques, primarily based upon Raman spectroscopy, are being developed and used to study high-temperature deposition and corrosion of materials exposed to combustion environments. Emphasis is on the 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. In situ analyses can be obtained with good temporal resolution (approximately ten spectra per second) for samples in high-temperature combustion environments. Both pulsed and continuous-wave lasers at various wavelengths throughout the visible and ultraviolet regions are available for excitation of Raman scattering, which can be detected with photon counting, gated integration, or optical multichannel techniques. Samples can be exposed to high-temperature corrosive environments in laboratory furnaces, which have optical access for in situ measurements. These experiments can likewise be performed with 1-2 micron resolution on a Raman microprobe, which has a hot stage for in situ studies. Also available are combustion flow reactors instrumented for Raman spectroscopy that provide a realistic environment for deposition and corrosion studies. Real-time measurements are complemented by post-exposure techniques such as Raman spectroscopy with sputtering and low-energy electron diffraction.

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 diagostic approaches for the study of material attack. In initiating collaborative research projects, it is desirable to perform preliminary Raman analyses of typical samples and of reference materials to determine the suitability of Raman spectroscopy to the user's particular application. Users interested in exploring potential collaborations should contact the persons listed below. If further investigations appear reasonable, a brief written proposal is requested. Generally, visits of a week or more for external users provide an optimum period for information exchange and joint research efforts. Users from industrial, university, and government laboratories have been involved in these collaborative efforts. Results of these research efforts are published in the open literature.

PERSONS TO CONTACT FOR INFORMATION

Marshall Lapp, High Temp. Interfaces Div. (8352) (415) 422-2435
FTS 532-2435

Gary B. Drummond, Ass't to the Director (8301) (415) 422-2697
FTS 532-2697

Sandia National Laboratories
Livermore, California 94550

TECHNICAL DATA

Instruments	Key Features	Comments
Raman Surface Analysis System	UHV Chamber; Raman system with Ar laser; triple spectrograph and array detector; Auger; sputtering capability.	Simultaneous Raman and sputtering. Raman system capable of detecting 2 nm thick oxides, up to 10 spectra per second. Sample heating up to 1100C.
Raman Microprobe	Hot stage; Raman system with Ar, Kr lasers; scanning triple spectrometer.	1-2 micron spatial resolution. Hot stage can handle corrosive gases.
Raman High-Temperature Corrosion System	Furnace; Raman system with Ar, Kr, Cu-vapor lasers; triple spectrograph and array detector.	Cavity-dumped Ar laser and Cu-vapor laser allow gated detection for blackbody background rejection. Fifty micron x 2 mm spatial resolution. Sample heating up to 1000C. Up to 10 spectra per second. Furnace allows exposure to oxidizing, reducing, and sulfidizing environments.
Combustion Flow Reactors	Raman system with Ar, Kr, Cu-vapor lasers; various spectrometers with PM tube and array detectors.	Burn various fuels. Vapor and particulate injection.
Raman Aqueous Corrosion System	Electrochemical cell; Raman system with Ar, Kr, Cu-vapor lasers; triple spectrograph and array detector.	Electrochemical cell with recirculating pump and nitrogen purge, up to 10 spectra per second.

MATERIALS PREPARATION CENTER

Ames Laboratory
Iowa State University
Ames, Iowa 50011

The Materials Preparation Center was established because of the unique capabilities for preparation, purification, fabrication and characterization of certain metals and materials that have been developed by investigators at the Ames Laboratory during the course of their basic research. Individuals within the Laboratory's Metallurgy and Ceramics Program are widely recognized for their work with very pure rare-earth, alkaline-earth and refractory metals. Besides strengthening materials research and development at the Ames Laboratory, the Center increases awareness by the research community of the scope and accessibility of this resource to universities, other government and private laboratories and provides appropriate transfer of unique technologies developed at the Center to private, commercial organizations.

Through these research efforts at Ames, scientists are now able to acquire very high-purity metals and alloys in single and polycrystalline forms, as well as the sophisticated technology necessary to satisfy many needs for special preparations of rare-earth, alkaline-earth, refractory and some actinide metals. The materials in the form and/or purity are not available from commercial suppliers, and through its activities the Center helps assure the research community access to materials of the highest possible quality for their research programs.

The Center consists of a Materials Preparation Section, an Analytical Section 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, MRSH Manager, (515) 294-8900 or FTS 865-8900.

TECHNICAL DATA

Materials

Scandium	Titanium	Magnesium	Thorium
Yttrium	Vanadium	Calcium	Uranium
Lanthanum	Chromium	Strontium	
Cerium	Manganese	Barium	
Praseodymium	Zirconium		
Neodymium	Niobium		
Samarium	Molybdenum		
Europium	Hafnium		
Gadolinium	Tantalum		
Terbium	Tungsten		
Dysprosium	Rhenium		
Holmium			
Erbium			
Thulium			
Ytterbium			
Lutetium			

PERSON TO CONTACT FOR INFORMATION

Frederick A. Schmidt, Director
Materials Preparation Center
121 Metals Development Building
Ames Laboratory
Ames, Iowa 50011

(515) 294-5236
FTS 865-5236

NATIONAL CENTER FOR ELECTRON MICROSCOPY

Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

The National Center for Electron Microscopy (NCEM) was formally established in fall 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, and a 1.6-MeV Kratos microscope dedicated largely for in situ work, a 1-MeV JEOL atomic resolution microscope (ARM), and a high-resolution feeder microscope (JEOL 200 CX). A 200-kV analytical microscope was recently installed. 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, A. Thomas, 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 of sufficient merit can be carried out as a collaborative effort between a Center postdoctoral fellow, the outside proposer, and a member of the Center staff.

PERSON TO CONTACT FOR INFORMATION

Ms. Madeline Moore
National Center for Electron Microscopy
Mail Stop: 72-131
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

(FTS) 451-5006, or
(415) 486-5006

NATIONAL CENTER FOR ELECTRON MICROSCOPY

TECHNICAL DATA

Instruments	Key Features	Characterization
KRATOS 1.5-MeV Electron Microscope	Resolution 3 Å (pt-pt) environmental cell; hot, cold stages.	50-80 hrs/week 150-1500 kV range in 100 kV steps and continuously variable. Max. beam current 70 amp/cm_2. 3-mm diameter specimens.
JEOL 1-MeV Atomic Resolution Microscope	Resolution < 1.7 Å (pt-pt) over full voltage range. Ultrahigh resolution goniometer stage, +40 Å biaxial tilt with height control.	50-80 hrs/week, 400 kV--1 MeV, LaB_6 filament, 3-mm diameter specimens.
Hitachi 650-kV Electron Microscope	General purpose resolution 20 Å environmental cell straining stage.	Installed in 1969. Max voltage 650 kV conventional HVEM, 3-mm diameter specimens.
JEOL 200 CX Electron Microscope	Dedicated high-resolution 2.4 Å (pt-pt) U.H. resolution goniometer stage only.	200 kV only, LaB_6 filament, 2.3-mm or 3-mm diameter specimens.
200-kV dedicated Analytical Electron Microscope	Microdiffraction, CBED, UTW X-ray detector, high-angle X-ray detector, EELS spectrometer.	100 kV--200 kV LaB6 filament, state-of-the-art resolution; 3-mm diameter specimens.

NATIONAL LOW-TEMPERATURE NEUTRON IRRADIATION FACILITY

Solid State Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

The National Low-Temperature Neutron Irradiation Facility (NLTNIF) will be a user-oriented facility for the study of radiation effects in materials. Currently under construction, it will be available for qualified experiments at no cost to users, beginning early in FY 1986. The NLTNIF will provide 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 will allow samples to be held at temperatures between 3.5 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 will be carried out in the irradiation cryostat. Alternatively, cold transfer to auxiliary equipment will be available. The conditions available in the NLTNIF 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 NLTNIF will be 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 will be assigned on the basis of proposals submitted in advance. Staff members will be aided in the selection of experiments by an advisory/program committee. Because of the special safety requirements of operating in a reactor, acceptance of proposals will require an evaluation by appropriate ORNL safety personnel in addition to the usual evaluation for scientific merit. Use of the reactor and cryostat will be at no cost to users, but extensive use of shops and other support facilities must be paid by the user.

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NATIONAL LOW-TEMPERATURE NEUTRON IRRADIATION FACILITY

Technical Data

Specifications of the cryostat and refrigeration system will be available after performance tests during the first 2-3 months in FY 1986. Neutronics characterization will be an ongoing facet of operations. Preliminary estimates of a few crucial properties are given here:

Refrigeration: Minimum temperature 3.5 K; Capacity at 5 K, 200 W
Radiation: Fast neutrons ($E > 0.1$ MeV) 2×10^{17} n/m^2s
Thermal neutrons 1.5×10^{17} n/m^2s
Gamma rays 0.3 W/g (in Al)
Dimensions of irradiation chamber: 4 cm diam by 25 cm length

SECTION F

Summary of Funding Levels

SUMMARY OF
FUNDING LEVELS

During the fiscal year ending September 30, 1985, the Materials Sciences total support level amounted to about $133.1 million in operating funds (budget outlays) and $15.5 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

	Contract and Grant Research (% by $)	Total Program (% by $)
(a) Northeast..... (CT, DC, DE, MA, MD, ME, NJ, NH, NY, PA, RI, VT)	42.2	28.6
(b) South..... (AL, AR, FL, GA, KY, LA, MS, NC, SC, TN, VA, WV)	10.0	19.1
(c) Midwest..... (IA, IL, IN, MI, MN, MO, OH, WI)	23.1	28.2
(d) West..... (AZ, CO, KS, MT, NE, ND, NM, OK, SD, TX, UT, WY, AK, CA, HW, ID, NV, OR, WA)	24.7	24.1
	100.0	100.0

2. By Discipline:

	Contract and Grant Research (% by $)	Total Program (% by $)
(a) Metallurgy, Materials Science, Ceramics (Budget Activity Number 01-)	58.6	37.2
(b) Physics, Solid State Science, Solid State Physics (Budget Activity Numbers 02-)	34.0	52.5

SUMMARY OF
FUNDING LEVELS

	Contract and Grant Research (% by $)	Total Program (% by $)
(c) Chemistry, Chemical Eng. (Budget Activity Numbers 03-)	7.4	10.3
	100.0	100.0

3. By University, DOE Laboratory, and Industry:

	Total Program (% by $)
(a) University Programs (including laboratories where graduate students are involved in research to a large extent, i.e., LBL, Ames and IL)...	35.0
(b) DOE Laboratory Programs.....	63.4
(c) Industry and Other.....	1.6
	100.0

4. By Laboratory and Contract and Grant Research:

	Total Program (%)
Ames Laboratory	5.8
Argonne National Laboratory	15.8
Brookhaven National Laboratory	20.5
Idaho National Engineering Laboratory	0.3
Illinois, University of (Materials Research Laboratory)	2.6
Lawrence Berkeley Laboratory	10.0
Lawrence Livermore National Laboratory	1.2
Los Alamos National Laboratory	2.9
Oak Ridge National Laboratory	16.9
Pacific Northwest Laboratory	1.4
Sandia National Laboratory	3.2
Solar Energy Research Institute	0.3
Stanford Synchrotron Radiation Laboratory	0.9
Contract and Grant Research	18.2
	100.0

SUMMARY OF
FUNDING LEVELS

5. By Selected Areas of Research:

	% of Prorated Projects[a] (Total=398)	% of Program Funding[a] ($133.1 million)	% of Individual Projects[c] (Total=398)
Materials			
Ceramics (Crystalline)	17.0	14.0	24.0
Ferrous Alloys	6.5	4.6	17.6
Intermetallics	3.7	3.5	9.0
Polymers	5.1	2.8	7.8
Semiconductors	8.1	6.7	14.1
Technique			
Electron Microscopy (Technique Development)	3.5	2.8	7.5
Neutron Scattering	4.6	18.1	10.8
Synchrotron Radiation	5.3	13.9	10.6
Theory	13.9	9.1	35.9
Phenomena			
Catalysis	2.6	2.4	8.0
Corrosion	6.6	4.4	10.3
Diffusion	3.3	3.3	12.7
Processing Science/Synthesis[b]	16.5	12.5	30.0
Strength	9.4	5.7	17.8
Superconductivity	3.2	3.0	6.0
Environment			
High Temperature (> 1200°K)	3.5	3.3	7.5
Radiation	5.2	3.2	9.0
Sulfur-Containing Gases	1.8	1.5	2.5

[a]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.

[b]Based on projects indexed in Section G under coatings, materials, preparation, powder metallurgy, solidification, surface treatments, thin films, and welding.

[c] Percentage of sum of individual projects involving the designated area of materials research.

SECTION G

Index of Investigators, Materials, Techniques, Phenomena, and Environment

INVESTIGATORS

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INVESTIGATORS

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MATERIALS

Nitrides
013, 022, 023, 054, 120, 178, 202, 203, 206, 233, 264, 303, 339, 343
363, 372, 380, 397, 420, 460, 470, 498, 506, 510

Oxides: Binary
022, 041, 047, 055, 080, 117, 118, 144, 151, 156, 164, 171, 173, 180
201, 203, 206, 219, 223, 233, 235, 239, 245, 248, 247, 260, 292, 301
303, 317, 329, 331, 339, 340, 343, 353, 362, 363, 367, 368, 369, 370
371, 372, 373, 379, 384, 391, 397, 407, 412, 414, 424, 429, 440, 442
446, 447, 452, 458, 461, 465, 469, 480, 492, 497, 498, 503, 504, 507
509, 512, 514, 516

Oxides: Non-Binary, Crystalline
022, 044, 050, 080, 116, 117, 144, 148, 151, 153, 160, 233, 235, 239
248, 260, 263, 292, 304, 317, 331, 334, 339, 348, 351, 363, 370, 372
379, 391, 393, 412, 414, 424, 425, 431, 444, 497, 504, 512, 504

Polymers
023, 078, 129, 180, 182, 204, 206, 228, 236, 240, 246, 255, 279, 295
307, 325, 342, 346, 353, 354, 356, 392, 415, 417, 418, 435, 443, 445
474, 484, 487

Platinum Metal Alloys (Platinum, Palladium, Rhodium, Irridium, Osmium, Ruthenium)
003, 016, 126, 142, 149, 291, 320, 350, 386, 432, 456, 461, 463, 473

Quantum Fluids and Solids
014, 047, 053, 125, 165, 170, 207, 227, 314, 322, 325, 330, 347, 358
376, 386, 492, 506

Radioactive Waste Storage Materials (Hosts, Canister, Barriers)
116, 200, 263, 304, 315, 372, 393, 425, 433, 461

Rare Earth Metals and Compounds
001, 003, 006, 007, 009, 011, 012, 015, 016, 019, 049, 053, 076, 080
170, 227, 229, 239, 244, 337, 386, 388, 394, 396, 462, 481, 483, 485
506

Refractory Metals (Groups VB and VI B)
004, 005, 007, 008, 011, 016, 017, 019, 022, 024, 040, 043, 073, 079
112, 140, 172, 175, 191, 232, 235, 238, 302, 317, 352, 401, 457, 514

Semiconductor Materials - Elemental (including doped and amorphous phases)
013, 070, 079, 120, 122, 140, 152, 161, 162, 163, 164, 168, 173, 177
180, 231, 234, 238, 241, 243, 275, 280, 298, 321, 338, 339, 357, 389
399, 400, 401, 437, 458, 462, 470, 515, 518, 511

Semiconductor Materials - Multicomponent (III-Vs, II-VIs, including doped and amorphous forms)
013, 018, 019, 108, 119, 122, 127, 128, 161, 162, 179, 231, 277, 280
296, 312, 339, 350, 384, 391, 399, 400, 403, 411, 414, 446, 469, 478
480, 504, 515, 518, 501

TECHNIQUES

PHENOMENA

ENVIRONMENT

Vacuum: High (better than 10**9 Torr)
011, 015, 050, 051, 052, 058, 084, 122, 180, 192, 203, 278, 350, 360
366, 411, 432, 457

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