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Materials Sciences Programs
Fiscal Year 1984

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 1984 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 1984 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]

- High Pressure Science and Technology (1983)
- Scientific Needs of the Technology of Nuclear Waste Containment (1983)
- Materials Preparation and Characterization Capabilities (1983)
- Critical and Strategic Materials (1983)
- Radiation Effects (1982)
- 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]
- Organic Conducting Materials[b]
- Coatings and Surface Modifications[c]
- Novel Methods for Materials Synthesis[b]
- Theory and Computer Simulation o Materials Structures and Imperfections[b]

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

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

Description of Research Facilities

- Centers for Collaborative Research[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.

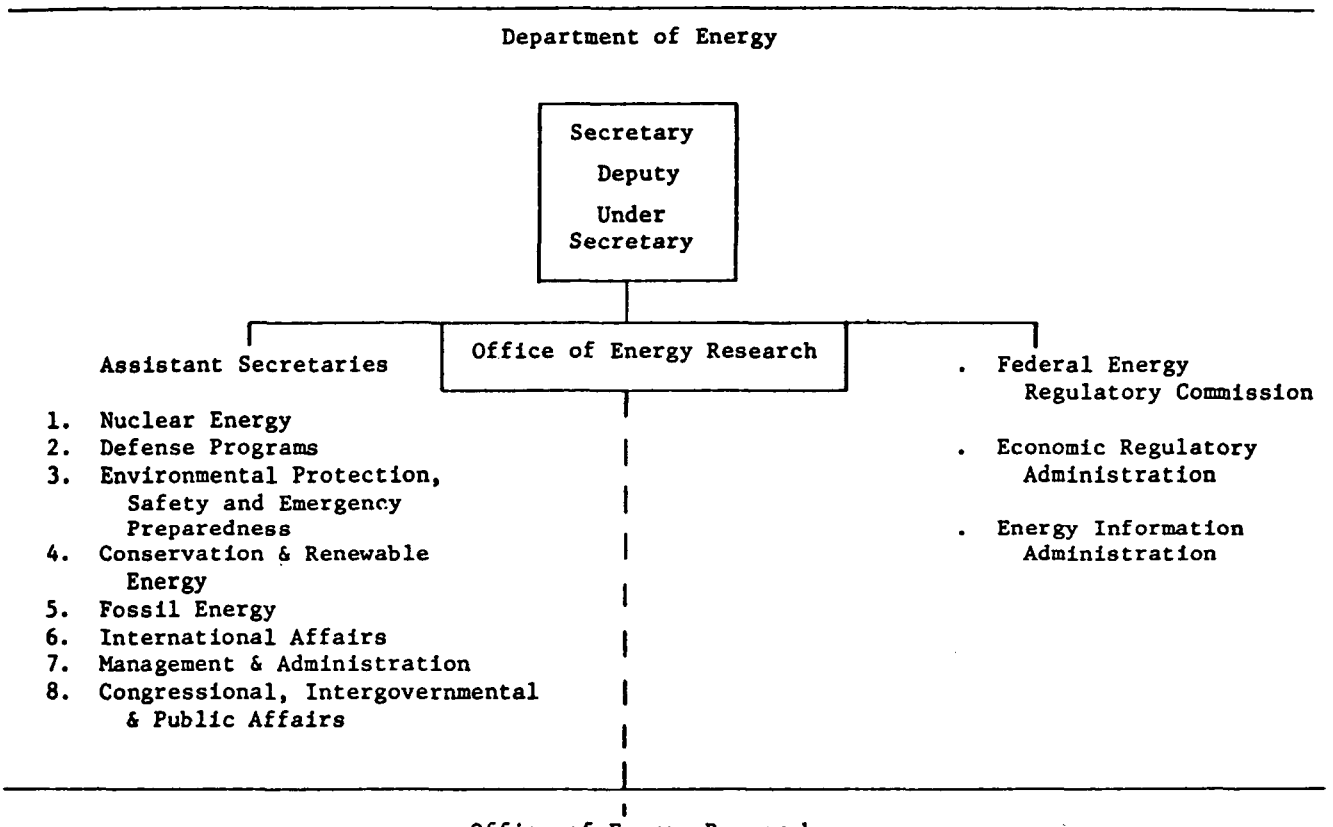
Winners of the 1984

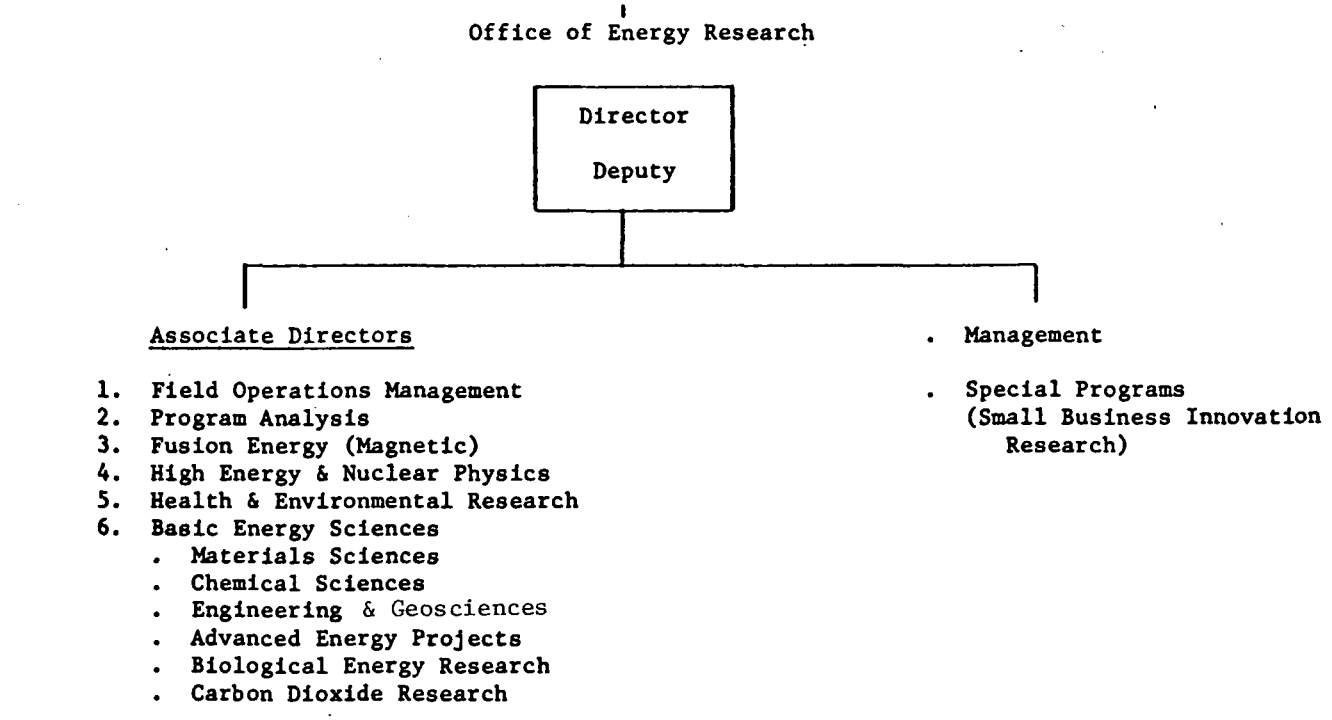
Materials Sciences Research Competition
Within the DOE Laboratories

Category	Winner(s)	
Metallurgy and Ceramics:		
o Outstanding Scientific Accomplishment	H. K. Birnbaum and I. M. Robertson, Univ. of Illinois, "Mechanisms of Hydrogen Embrittlement"	ILL
o Sustained Outstanding Research	P. Okamoto, L. Rehn, H. Wiedersich, N. Lam, and R. Averback, ANL, "Radiation-Induced Segregation"	ANL
o Significant Implication for Energy Technology	C. T. Liu, C. L. White, and J. A. Horton, ORNL, "Design of Ductile Nickel Aluminides for High Temperature Structural Use"	ORNL
Solid State Physics:		
o Outstanding Scientific Accomplishment	S. Chiang, P. L. Richards, and R. G. Tobin, LBL, "Infrared Emission Spectroscopy of Chemisorbed Molecules on Metal Surfaces"	LBL
o Sustained Outstanding Research	C. P. Slichter, Univ. of Illinois, "Static and Dynamic Properties of Solids"	ILL.
o Significant Implication for Energy Technology	B. C. Sales and L. A. Boatner, ORNL, "Lead-Iron Phosphate Glass: A New Stable Storage Medium for High-Level Nuclear Waste"	ORNL
Materials Chemistry:		
o Outstanding Scientific Accomplishment	W. G. Breiland, M. E. Coltrin, and Pauline Ho, SNL-A, "Fundamental Mechanisms of Chemical Vapor Deposition (CVD)"	SANDIA/ A
o Sustained Outstanding Research	M. Blander, ANL, "Application of Thermodynamics to Materials Science"	ANL
o Significant Implication for Energy Technology	A. R. Krauss, ANL, "Self-Sustaining, Low-Z Coatings for Magnetic Confinement Fusion Applications"	ANL

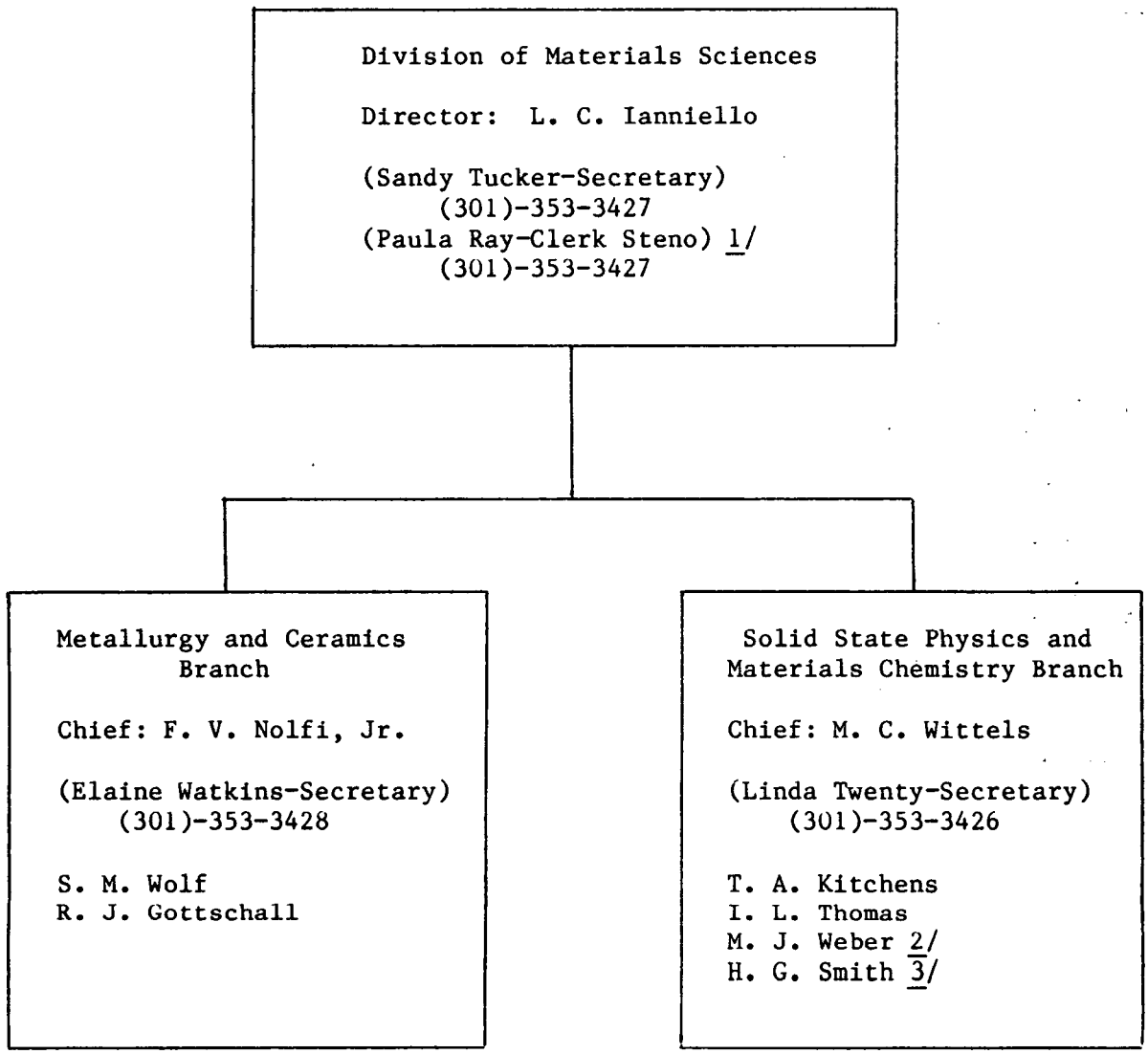
ANL	ORNL	LBL	ILL	S/A
3	2	1	2	1

ORGANIZATION OF THE DEPARTMENT OF ENERGY





OFFICE OF BASIC ENERGY SCIENCES, Division of Materials Sciences Structure



Notes: 1/ Temporary Assignment from Energy Research Administrative Office
2/ On Leave from Lawrence Livermore National Laboratory
3/ On Leave from Oak Ridge National Laboratory

INTRODUCTION

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

The report is divided into six sections. Section A contains all Laboratory projects, Section B has all contract research projects, Section C has projects funded under the Small Business Innovation Research Program, Section D has information on DOE collaborative research centers, Section E gives distributions of funding, and Section F 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 F. The FY 1984 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

Section D contains information on special DOE centers that are operated for collaborative research with outside participation. Section E 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 F 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 1984 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 Miss P. Kay and Mrs. L. Twenty, who also kept the effort on track. This year the Summary was done "by the computer." This could not have been accomplished without the very competent professional assistance of Mrs. K. Roskin, Calculon, Inc.

TABLE OF CONTENTS

SECTION A - Laboratories

SECTION B - Grant and Contract Research

SECTION C - Small Business Innovation Research

SECTION D - Collaborative Research Centers

SECTION E - Funding Levels

SECTION F - Index

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.

LABORATORIES

AMES LABORATORY
Iowa State University
Ames, Iowa 50011

Metallurgy and Ceramics - 01 -

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

001. MATERIALS SCIENCE OF INTERFACES

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

$202,000 01-1

Studies of interface structure and composition using Auger, ELS, and SIMS surface analytical techniques in combination with ion etching. Core level and plasmon spectra of pure rare earth metals using ELS and Auger. Auger spectroscopy of metallic hydrides for phase identification. Effects of tin alloying on brass corrosion behavior in aqueous salt solutions. Scanning Auger microprobe analysis (35nm) of grain boundary inclusions in carbonized low alloy steels and effects of radiation on the competition between C and P grain boundary segregation in iron. Local chemical state information from Auger lineshape analysis in Fe-B-Be metallic glasses.

002. NONEQUILIBRIUM MATERIALS

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

$255,000 01-1

Studies of metallic glasses, metastable crystalline phases and extremely fine microstructural alloys. Ultra high vacuum melt spinning apparatus to process reactive metals without contamination. Directional solidification apparatus modified to achieve extremely large undercooling and solidification rates. High speed planar solidification of eutectic Pd-Cd. Microstructural study by TEM of transformation products of decomposition of metallic glasses and of rapidly crystallized solids.

003. SURFACES AND SOLIDIFICATION

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

$206,000 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 materials such as succinonitrile and acetone mixtures. Microstructure development during amorphous to crystalline transition.

LABORATORIES

AMES LABORATORY (continued)

004. MICROSTRUCTURAL CONTROL IN METALS

J. D. Verhoeven, E. D. Gibson
Phone: (515)-294-9471

$297,000 01-1

Production of Nb_3Sn-Cu and V_3Ga-Cu superconducting wire by the in situ process, study of problems on the addition of Sn and Ga by the external diffusion method and evaluation of filament cross linking within the microstructure. A study of directionally transformed pearlite versus applied stress level and temperature gradient. The mechanical properties of in situ prepared Cu-base composite alloys. Directional solidification studies on segregation and morphology in grey, nodular and white cast iron. Evaluation of microstructural changes in the austempering of nodular cast irons. Microstructure evolution under solidification conditions typical of welding processes.

005. MECHANICAL METALLURGY

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

$400,000 01-2

Effects of hydrogen on crack initiation in refractory alloys under uniaxial and cyclic loading conditions. Hydrogen diffusion in vanadium base alloys by internal friction. Hydrogen induced brittle cracking in low hydrogen solubility bcc metals and alloys. Studies on the 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

$86,000 01-3

Development of thermodynamic functions for alloy formation in Y-Fe, Y-Co, and Y-Ni systems from electromotive force measurements to test the conflicting predictions of the Bennett-Watson theory and the Miedema theory. Computer analysis of thermodynamic data for the prediction of stable and metastable phase equilibria, metallic glass formation, and control of microstructures.

LABORATORIES

AMES LABORATORY (continued)

007. TRANSPORT STUDIES

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

$190,000 01-3

Study of fast diffusion and electrotransport of metallic solutes in scandium and thorium. Measurement of transport parameters for iron, in scandium and cobalt thorium as a function of temperature and determination of activation energies for diffusion. Investigation of mechanism and type of defect responsible for fast diffusion of cobalt in thorium by use of internal friction and scanning electron microscopy. Thermotransport of interstitial solutes in vanadium-titanium alloys. Mass transport of carbon in two-phase Nb-C and V-C alloys in presence of temperature gradient. Precise determination of solid solubility of carbon in vanadium.

008. HYDROGEN IN METALLIC SOLIDS

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

$257,000 01-3

Diffusion, thermotransport, and solubility of H and D in V alloys with Ti, Cr, 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

$252,000 01-3

The influence of composition and impurities on the 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 $CeSn_x$ ($x \sim 3$) and $CeSi_x$ ($x \sim 1.8$) alloys; and (3) itinerant ferromagnets Sc_3In and $ZrZn_2$. Low temperature (1-20 K) - high magnetic field (1-10 T) heat capacity, magnetic susceptibility (1-300 K, 0.9 to 1.5 T), resistance ratio ($\rho_{300}/\rho_{4.2}$), metallography and lattice parameters measurements are being used to characterize the various behaviors. Nonequilibrium phases resulting from solidification and phase transformations in rare earth based alloys.

LABORATORIES

AMES LABORATORY (continued)

010. NDE MEASUREMENT TECHNIQUES

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

$383,000 01-5

Techniques to measure failure related material properties are investigated. Dual objectives of improving understanding of failure mechanisms and inspection reliability. Ultrasonic measurement of internal stresses. Ultrasonic scattering and harmonic generation studies of fatigue cracks to provide detailed information about closure condition near crack tip and to determine the influence of this condition on detectability. Microscopic characterization and modeling of the effects of stress and deformation on crack initiation and growth of brass under corrosive conditions. Relationship between fatigue damage or stress on magnetic properties.

011. PROCESSING OF CERAMICS

M. Akinc, G. W. Jordan, M. D. Rasmussen
Phone: (515)-294-6964

$252,000 01-5

Effect of processing variables on characteristics of ceramic powders. Influence of hydroxide precursor dewatering treatments on morphology, surface characteristics, compaction and sintering behavior of oxide powders produced from them.

012. ADVANCED MATERIALS AND PROCESSES (see also page D-25)

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

$170,000 01-5

Processing of refractory and strategic metals. New process for preparing kilogram quantities of high purity vanadium. Development of arc melting procedures for preparing Cu-Nb, Cu-Ta and Cu-Mo alloys containing uniform dispersion of the refractory metal. Processing of stoichiometric and non-stoichiometric materials by an inductively coupled plasma. Measurement of diffusion and electrotransport behavior of solutes in rare-earth and refractory metals and the application of these parameters for maximum purification of the host metals. Processing of single crystals of pure metals, solid solution alloys, and intermetallic compounds, both congruent melting and peritectic in nature, by levitation zone melting in cold crucible, 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.

LABORATORIES

AMES LABORATORY (continued)

Solid State Physics Division - 02 -

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

013. NEUTRON SCATTERING

W. A. Kamitakahara, J. Mizuki, C. Stassis, J. Zarestky
Phone: (FTS) 865-4224 or (515)-294-4224
$360,000 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, $YbAl_2$); relation of electron-phonon interaction to superconductivity (La, $LaSn_3$). High pressure studies (α-Ce, La).

014. SEMICONDUCTOR PHYSICS

H. R. Shanks
Phone: (FTS) 865-6816 or (515)-294-6816
$200,000 02-2

Preparation and characterization of thin films, rf sputter desposition of amorphous semiconductors including aSi, aSi-C, aGe, aGe-C and AlN, ionized cluster beam and deposition of Si, heteroepitaxy on compound substrates, 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.

015. SUPERCONDUCTIVITY

D. K. Finnemore, J. R. Ostenson, E. L. Wolf, T. P. Chen, Y. Q. Zhou
Phone: (FTS) 865-3455 or (515)-294-3455
$430,000 02-2

Electron tunneling spectroscopy and surface physics studies of strong coupled transition metal superconductors, including alloys and compounds. Conventional and 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 inhomogeneous materials; use of Josephson junctions to study flux pinning of isolated vortices, development of materials with very low pinning, and studies of the motion quantized vortices in SNS junctions; 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.

Stoughton, Wisconsin 608-873-6651

LABORATORIES

AMES LABORATORY (continued)

016. OPTICAL AND SPECTROSCOPIC PROPERTIES OF SOLIDS AND LIQUIDS

D. W. Lynch, C. G. Olson, D. M. Wieliczka
Phone: (FTS) 865-3476 or (515)-294-3476
$290,000 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., $CeSn_3$), Fe-based alloys with Si and Al, amorphous SiC, benzotriazol on Cu; electroreflectance of emersed Ag electrodes, photon- and electron-stimulated desorption of neutral atoms from insulators.

017. NEW MATERIALS AND PHASES

R. N. Shelton, C. A. Swenson, R. G. Barnes, M. S. Anderson, P. Klavins, D. R. Torgeson
Phone: (FTS) 865-5435 or (515)-294-5435
$520,000 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 and 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 (alkali and alkaline earth metals); effects of hardness on thermal expansivities of technical materials (beryllium copper); low temperature expansivity of materials (Lu) containing hydrogen. Applications of NMR to hydrogen embrittlement of refractory metals (V, Nb, Ta) and alloys (V-Ti, Nb-V), trapping of hydrogen by interstitial impurities in these metals, structural and electronic characterization of hydrogenated amorphous Si, Ge, SiC, and GeC films.

LABORATORIES

AMES LABORATORY (continued)

018. MATERIALS FOR HYDROGEN STORAGE

R. G. Barnes, J. D. Corbett, K. A. Gschneidner Jr.,
W. A. Kamitakahara, D. T. Peterson
Phone: (FTS) 865-4754 or (515)-294-4754; (515)-294-1560

$185,000 02-2

Interdisciplinary study of metal-hydrogen interactions for development of better hydrogen-storing materials. Materials studied include hydrides of transition metals (e.g., YH_2), refractory alloys (e.g., V-Ti-H), rare-earth-transition metal compounds (e.g., $Y(Al,Ni)_5$-H), and low-valent and lower-dimensional compounds of Group III and IV metals (e.g., LaCl-H, ZrCl-H). Properties and methods include hydrogen locations, super structures, phase transformation, electronic density-of-states, hydriding kinetics, enthalpies of hydride formation, hydrogen diffusion, low-temperature heat capacity, X-ray and neutron diffraction, nuclear magnetic resonance, XPS and UPS.

019. X-RAY DIFFRACTION PHYSICS

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

$235,000 02-2

X-ray diffraction studies of semiconducting compounds, epitaxial layers, and superlattices. X-ray studies of La at high pressures. Electron charge density studies of V_3Si and Fe-Ni-C in the vicinity of the martensitic phase transition. MATRIX PRT beam line at NSLS.

020. ELECTRONIC AND MAGNETIC PROPERTIES

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

$410,000 02-3

Theory of phonon anomalies, lattice instabilities and soft modes in metals and their relation to the electron-phonon interaction and superconductivity (Nb, Mo, Zr, Ti). Total energy frozen phonon calculations for high temperature bcc to ω-phase transition and lattice dynamics. Surface electronic structure of metal electrodes (e.g., Ag), electroreflectance, and microscopic properties of the metal-electrolyte interface. Static and dynamic properties of mixed valence compounds ($CeSn_3$). Electronic properties and chemical bonding of transition and rare-earth metal compounds (ZrB_2, $ZrSe_3$, ZrS, TiS, PtTe, LaH_2, LaH_3, ScH_2). Vacancy formation and ordering (Sc_xS). Renormalization group studies of phase transitions. Electron localization in disordered metals.

LABORATORIES

AMES LABORATORY (continued)

021. OPTICAL AND SURFACE PHYSICS THEORY

R. Fuchs, K.-M. Ho, S. Auluck
Phone: (FTS) 865-3675 or (515)-294-3675
$160,000 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 and reconstruction at single crystal surfaces (Al, Au).

022. SUPERCONDUCTIVITY THEORY

J. R. Clem, V. G. Kogan
Phone: (FTS) 865-4223 or (515)-294-4223
$120,000 02-3

Electrodynamics of superconductor-normal metal composites; properties of current-carrying type-I and type-II superconductors containing magnetic flux; induced voltages and energy dissipation due to flux motion; vortex nucleation and surface pinning; flux-line cutting in arrays of nonparallel vortices; critical currents and flux pinning in inhomogeneous superconductors; ac losses; two-dimensional Josephson junction arrays; superconducting magnetic shielding.

LABORATORIES

AMES LABORATORY (continued)

Materials Chemistry Division - 03 -

L. E. Burkhart - Phone (FTS) 865-8074 or 515-294-8074

023. X-RAY AND NEUTRON CRYSTALLOGRAPHY

R. A. Jacobson, B. J. Helland
Phone: (515)-294-8444

$185,000 03-1

Determination of atomic arrangements in crystalline and non-crystalline materials by x-ray and neutron diffraction, and EXAFS spectroscopy. 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. Atom-atom pair correlation functions for non-crystalline materials. Materials studied include rare-earth superconductors, model homogeneous catalysts, polymetal species, complex molybdates, and sulfides, and other substances where intramolecular solid state interactions can modify properties of the parent species.

024. SYNTHESIS AND CHARACTERIZATION OF NEW MATERIALS

J. D. Corbett
Phone: (515)-294-3086

$175,000 03-1

Synthesis, structure and bonding in intermetallic systems - new Zintl phases, new ternary compounds showing bonding of the type found in A15 phases, interstitials. Reactions and stabilities of phases in the system CsI-Zr-ZrI_2-ZrO_2, effects of common impurities, the fate of the important fission products. Low temperature routes to rare-earth oxychlorides and their application to oxygen removal from metals. Properties of metal structures stabilized by interstitial nonmetals including hydrogen. Techniques include high temperature reactions, phase equilibria, transport and crystal growth in inert metal containers, X-ray diffraction, bonding studies by photoelectron spectroscopy, extended Huckel calculations.

LABORATORIES

AMES LABORATORY (continued)

025. CHEMISTRY OF HEAVY TRANSITION METALS

R. E. McCarley
Phone: (515)-294-8680

$170,000 03-1

Synthesis, structure and properties of new ternary oxide phases containing heavy transition elements, especially reduced compounds with metal-metal bonded structures stable at high temperatures. Study of new oxide materials having low dimensional electrical properties, framework, or layer structures which promote high cation mobility for ion-exchange and ionic conductivity, and one-dimensional growth for high strength fibrous ceramics. Correlation of structure and bonding with d-electron count, and relations between structure and physical properties. Experimental methods include X-ray diffraction, photoelectron spectroscopy, resistivity measurements, tensile strength measurements, Mossbauer spectroscopy, and nuclear magnetic resonance.

026. PARTICULATE PROCESSING

L. E. Burkhart, A. Cahill
Phone: (515)-294-8074

$305,000 03-2

Preparation and characterization of ceramic powders with emphasis on liquid-phase methods. Control of nucleation, growth, agglomeration, and morphology to produce powders that sinter to high densities. Quantitative characterization of agglomerates (mechanisms, strength distributions) and correlation with sintering behavior. Theoretical studies include DLVO theory for particle-particle interactions, coagulation and population balance equations for agglomeration kinetics, and Fourier and fractal analysis for morphology. Experimental techniques used are SEM-TEM microscopy, BET surface areas, X-ray diffraction, mercury porosimetry, and image analysis.

027. CARBOTHERMAL PROCESSING OF NON-OXIDE CERAMICS

G. Burnet, M. J. Murtha
Phone: (515)-294-5840

$185,000 03-2

Investigation of reaction mechanisms and kinetics of the preparation of ceramic powders by carbothermal processing, with emphasis on silicon nitride and silicon nitride-based materials. Experimental methods include the use of direct-coupled electrobalance and gas chromatography systems.

LABORATORIES

AMES LABORATORY (continued)

028. HIGH TEMPERATURE CHEMISTRY OF REFRACTORY MATERIALS

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

$255,000 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.

029. SURFACE CHEMISTRY AND CATALYSIS

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

$335,000 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. Variation of surface intermediates with surface morphology and of surface reactivity with surface structure. 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.

LABORATORIES

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

Materials Science and Technology Division

F. Y. Fradin - Phone (FTS) 972-4925 or 312-972-4925
H. Wiedersich (01) - Phone (FTS) 972-5079 or 312-972-5079
M. B. Brodsky (02) - Phone (FTS) 972-5016 or 312-972-5016
D. M. Gruen (03) - Phone (FTS) 972-3513 or 312-972-3513

Intense Pulsed Neutron Source Program

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

040. DEFECTS IN METALS

R. W. Siegel, R. Benedek, M. J. Fluss, N. Q. Lam, J. N. Mundy, J. E. Robinson, L. C. Smedskjaer, D. G. Westlake, R. Prasad
Phone: (312)-972-4963

$1,408,000 01-3

Research on the nature and physical properties of intrinsic and extrinsic atomic defects and their interactions in metals and alloys, and the relationship between these and the atomic mechanisms of diffusion under equilibrium and non-equilibrium conditions and the properties of metallic materials; investigations of atomic and defect diffusivities; equilibrium defect formation and concentrations; interactions of atomic defects with one another, with solute atoms, and with interfaces and surfaces; hydrogen interactions with metallic systems; studies of metals (with emphasis on refractory bcc metals), alloys, intermetallic compounds, and amorphous metallic systems with experimental techniques such as positron annihilation spectroscopy, radio-tracer diffusion, resistometry, perturbed angular correlation, transmission and scanning electron microscopy, neutron and x-ray diffraction, and ion-scattering spectroscopy, and the complementary theoretical methods of molecular statics and dynamics, computer modeling, and electronic structure calculations.

Henry Thomas 5023

LABORATORIES

ARGONNE NATIONAL LABORATORY (continued)

041. DEFECTS IN CERAMICS

N. L. Peterson, K. L. Merkle, G. E. Murch, J. L. Routbort, D. Wolf, K. Hoshino, M. P. Thomas
Phone: (312)-972-4955

$848,000 01-3

Diffusion mechanisms and point-defect studies in metal oxides as a function of oxygen partial pressure at high temperatures using cation and oxygen tracer diffusion, conductivity and TEM techniques; impurity diffusion mechanisms, defect-solute interactions and defect clustering in oxides; computer modeling of diffusion processes at dislocations and in non-stoichiometric compounds; TEM studies of dislocation structures in grain boundaries in oxides; theory of defect kinetics, vibration entropy, and atomic structure in grain boundaries; grain boundary diffusion in metal oxides; diffusion mechanisms and impurity interactions in mixed-alkali silicate, alkali borate, alkali germanate, alkali-germanium-sulfur, and alkali-silicon-sulfur glasses; effect of nonstoichiometry and defect clusters on mechanical deformation of oxides; preparation of single and bicrystals of metal oxides.

042. NEUTRON IRRADIATION STUDIES

M. A. Kirk, R. C. Birtcher, B. A. Loomis
Phone: (312)-972-4998

$434,000 01-4

Fast neutron irradiation effects in solids studied using the Radiation Effects Facility at IPNS and in-situ ion irradiation in the HVEM facility; structure and properties of cascades, interactions of free interstitials and vacancies and their clusters in metals and alloys using resistivity, ordered alloys, TEM, and electron irradiation probe techniques; interactions of gliding dislocations with neutron irradiation produced defect structures studied in the HVEM in niobium, vanadium and their alloys; the collapse of defect cascades to dislocation loops studied in the HVEM in Cu_3Au and Fe following low temperature in-situ ion irradiatons; low temperature defect production and annealing in semiconductors studied with resistivity and deep level transient spectroscopy; superconducting property changes in various metallurgical states of Nb-Ti following fast neutron irradiation at 5K; changes in mechanical properties of organic composite insulators following fast neutron irradiations at 5 and 300 K.

LABORATORIES

ARGONNE NATIONAL LABORATORY (continued)

043. IRRADIATION AND KINETIC EFFECTS

L. E. Rehn, R. S. Averback, S. Majumdar, P. R. Okamoto,
R. B. Schwarz, N. J. Zaluzec, J. Don, J. Mansfield, D. Peak
Phone: (312)-972-5021

$1,135,000 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; effects of irradiation on alloy composition and microstructure; in-situ studies of ion and electron bombardment in the High Voltage Electron Microscope; mechanistic studies of deformation and mechanical strengthening in alloys; ion-beam analysis, analytical electron microscopy; radiation sources include HVEM-2MV Tandem facility and two 300 kV ion accelerators.

044. ELECTRON MICROSCOPY CENTER FOR MATERIALS RESEARCH (see also page D-15)

A. Taylor, R. W. Siegel, N. J. Zaluzec
Phone: (312)-972-5109

$666,000 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; 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 Analytical Electron Microscope is being acquired; 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)

045. OXIDATION STUDIES

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

$658,000 01-5

Point defects and diffusion mechanisms in protective-oxide scales; grain-boundary diffusion in pure and doped protective-oxide materials; studies of adhesion and morphology of oxide scales on crystalline and amorphous alloys using analytical-electron-microscopy techniques; mechanisms and kinetics of oxide film breakdown in bioxidant atmospheres.

046. AMORPHOUS METALLIC ALLOYS

R. B. Schwarz, T. I. Morrison, D. G. Westlake
Phone: (312)-972-4979

$150,000 01-5

Investigations of the synthesis of amorphous metallic materials by isothermal solid-state reactions at the interfaces of vacuum-deposited pure metallic films and mechanically alloyed powders, and by hydrogenation/dehydrogenation reactions; X-ray diffraction, electron microscopy, and Rutherford backscattering studies of the morphology and kinetics of the crystalline-to-amorphous transformation; investigations of the relationships between the atomic structure of amorphous alloys and their magnetic, mechanical and corrosion properties; consolidation of amorphous powders by hot pressing and dynamic compaction.

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, M. Arai, R. O. Hilleke, C. K. Saw, M. H. Mueller
Phone: (312)-972-5475

$1,465,000 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-I and NSLS. Investigations of the structure and defects of ternary superconductors; chalcogenide, oxide, and silicate glasses; surface magnetism; alloy mixing produced by neutron irradiation; residual stresses in deformed materials; decomposition of binary alloys; nuclear magnetic ordering; excited states of hydrogen in metals; magnetism in rare-earth noble-metal compounds; atomic momentum distributions with deep inelastic scattering; mixed conducting lithium electrodes.

ARGONNE NATIONAL LABORATORY (continued)

048. CHEMICAL AND ELECTRONIC STRUCTURE

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

$949,000 02-1

New materials synthesis and characterization focussing on synthetic organic metals, organic superconductors, dielectric materials, and organometallic compounds that behave as model catalysts or catalysts; development of structure-property relationships, and electrical properties measurements, of synthetic metals based on TMTSF (tetramethyltetraselenafulvalene) and BEDT-TTF bis(ethylenedithiotetrathiofulvalene); continuing development of the neutron time-of-flight single-crystal diffractometer (SCD), and the associated U.S. university-industrial users group, at the Intense Pulsed Neutron Source; diffuse scattering and crystal structure studies at the SCD as a function of temperature (10-300 K); development of a facility for single crystal X-ray studies centered around a low temperature (10 K) X-ray instrument for electron density and structural studies.

049. INTENSE PULSED NEUTRON SOURCE PROGRAM (see also page D-7)

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

$4,900,000 02-1

The IPNS Program has the goal of providing an intermediate-flux pulsed spallation neutron source for condensed matter research with neutron scattering and irradiation techniques. The IPNS facility is equipped with 7 instruments which are regularly scheduled for users and 3 beam tubes which are assigned to special experiments. Routine operation started in November 1981. The facility is run as a national facility in which experiments are selected on the basis of scientific merit by a nationally constituted Program Committee. Approximately 110 experiments, many involving participants in collaborative research from Universities and industry were performed in the period October 1981-October 1983 and another 60 will be scheduled for the next 6 months. Industrial Research on a proprietary basis, which allows the company to retain full patent rights, has been initiated with a number of companies (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.

LABORATORIES

ARGONNE NATIONAL LABORATORY (continued)

050. SUPERCONDUCTIVITY AND MAGNETISM

B. D. Dunlap, G. W. Crabtree, K. E. Gray, D. G. Hinks,
H. A. Kierstead, T. I. Morrison, G. K. Shenoy, H. Aoki,
A. J. Fedro, W. P. Joss, S. K. Malik, B. D. Terris, A. M. Umarji
Phone: (312)-972-5538

$1,391,000 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 and narrow-band materials containing rare-earth and actinide elements; 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.

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

S. Susman, T. O. Brun, K. Kuriyama
Phone: (312)-972-5470

$464,000 02-2

Preparation of metal, insulator and semiconductor single crystals with documented physical and chemical properties; solidification of vitreous systems with characterized and reproducible compositions and thermal histories; investigations of mechanisms involved in purification, crystal growth, phase transformations and solidification; materials of current interest include semiconducting chalcogenide glasses, Zintl-phase compounds, complex aluminosilcates and cyanides; basic studies conducted in the microscopics of charge and mass transport in solid electrode and electrolyte materials utilizing X-ray diffraction, nuclear magnetic resonance, ionic conductivity, EXAFS, and optical spectroscopy; fast ion transport examined in mixed electronic and ionic conductors and in fast-ion glasses; these include Li-Al alloys, NASIGLAS, and both crystalline and vitreous eucryptites.

LABORATORIES

ARGONNE NATIONAL LABORATORY (continued)

052. ELECTRONIC STRUCTURE AND BONDING

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

$1,500,000 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 actinide oxides in silicate glasses; crystal chemistry and structural phase transformation studies of complex metal oxides using X-ray diffraction and electron microscopy; XPS and XANES studies of structural and electronic properties of ABO_4 compounds; 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 XPS) studies of actinide intermetallic compounds to determine the electronic configuration and stability of 5f electron states.

053. LAYERED AND THIN FILM MATERIALS

I. K. Schuller, S. D. Bader, M. B. Brodsky, M. Grimsditch, C. S. L. Chun, L. Sill, G. W. Zajac
Phone: (312)-972-5469

$946,000 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, 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)

054. CONDENSED MATTER THEORY

D. Y. Smith, L. Guttman, R. Kalia, D. Koelling, A. Rahman, P. Vashishta, K. Lee, M. Norman, M. Schneider
Phone: (312)-972-5481

$902,000 02-3

Condensed matter theory focusing on statistical physics, electronic structure, and the defect solid state. Current areas of study include: molecular-dynamics modeling of structural phase transitions, melting and nucleation, and fast ion transport in solids; electronic structure calculations of organic superconductors and narrow-band materials, including actinides and mixed-valence systems; many-body effects, especially Green's function Monte Carlo simulation of multi-exciton complexes and the electron-hole liquid; optical and X-ray properties of materials; the electronic structure of defects in insulators and electron solvation in molten salts; calculations of the spatial and electronic structure of amorphous semiconductors and covalent glasses.

055. ULTRA-HIGH FIELD SUPERCONDUCTORS

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

$85,000 02-5

Development of magnetron sputtered films of superconducting materials such as 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 will be measured; material characterization by X-ray, EELS, RBS, and TEM; technique development for fabrication of continuous tapes and/or wires of stabilized NbN suitable for winding ultra-high field superconducting magnets.

056. GEOPHYSICAL PROSPECTING WITH SQUIDS

R. T. Kampwirth
Phone: (312)-972-5521

$100,000 02-5

Development of portable instrumentation system for data acquisition and analysis of extremely weak magnetic and electric fields using Superconducting QUantum Interference Devices (SQUIDs) and telluric electrodes for signal detection; both magnetotelluric and controlled source signal sources; applications include nonintrusive lithosphere mapping, and search for subsurface hydrocarbon and mineral deposits; especially useful in regions of high sound velocity (e.g., basaltic overflows) where no seismic sections are obtainable; instrumentation system being prepared for transfer to an institution doing geophysics research.

ARGONNE NATIONAL LABORATORY (continued)

057. THERMODYNAMICS OF ORDERED AND METASTABLE MATERIALS

M. Blander, R. Blomquist, L. A. Curtiss, H. E. Flotow, V. A. Maroni, P. A. G. O'Hare, M.-L. Saboungi
Phone: (312)-972-4548

$810,000 03-2

Experimental and theoretical studies of thermodynamic and structural properties of ordered solutions, amorphous (metastable) materials, strategic minerals, and chemical species that have significance for elevated-temperature corrosion processes; thermodynamic measurements (e.g., emf), structural (e.g., neutron diffraction) and theoretical (e.g., molecular dynamics) studies of solution behavior of ordered and associated liquids (e.g., chloroaluminates, ionic alloys, silicates); thermodynamic calculations based on statistical mechanics of complex metallurgical media as well as corrosion processes; electronic absorption spectroscopy, X-ray diffraction, proton activation, and cyclic voltammetry are used to explore the dissolution of metals contained in domestic minerals and in industrial/energy by-products; thermochemical measurements of enthalpies of formation, standard entropies, and Gibbs energies of formation of strategically important minerals, fiber optic materials, and fast ion conducting glasses; drop calorimetric and vapor pressure measurements on systems exhibiting metal-to-nonmetal transitions.

058. INTERFACIAL MATERIALS CHEMISTRY

V. A. Maroni, M. Blander, L. A. Curtiss, B. D. Holt, S. A. Johnson, R. Kumar
Phone: (312)-972-3513

$1,017,000 03-2

Experimental and theoretical investigations of interfacial processes that are important to corrosion science, catalysis, and atmospheric chemistry; studies of surface and near-surface gas/particle and gas/substrate interactions using attenuated total internal reflection (ATR) Fourier transform infrared spectroscopy; ATR and Auger/ESCA studies of bonding of absorbed species in the cavities of shape selective catalysts; Ab-initio quantum mechanical and classical statistical mechanical calculations of structure, bonding, and reaction energies with emphasis on surface absorbed species and atomic clusters; investigations of the mechanism of conversion of SO_2 to sulfates in the atmosphere using oxygen isotopic techniques and high-resolution tunable diode laser infrared spectroscopy.

LABORATORIES

ARGONNE NATIONAL LABORATORY (continued)

059. AQUEOUS CORROSION

V. A. Maroni, D. M. Gruen, C. A. Melendres, Z. Nagy, M. Pellin, R. M. Yonco
Phone: (312)-972-3513

$150,000 03-2

Fundamental aspects of aqueous corrosion with emphasis on mechanisms responsible for stress corrosion cracking (SCC) of iron and iron-based alloys at high temperatures and pressures (300°C, 100 atm); application of in-situ surface-sensitive spectroscopic techniques (laser Raman, Raman gain, second harmonic generation, surface extended X-ray absorption fine structure, and Auger/ESCA) in combination with transient electrochemical methods to unravel the details connecting surface adsorption/reaction initiation and grain boundary effects involved in SCC; supporting theoretical studies using (1) molecular dynamics methods to study interactions at the water-metal interface on the molecular level and (2) porous electrode theory to obtain a macroscopic description of the influence of water chemistry on the corrosion behavior of iron-based alloys.

060. PARTICLE-SURFACE INTERACTION CHEMISTRY AND CATALYSIS

D. M. Gruen, B. M. Abraham, W. F. Calaway, L. E. Iton, A. R. Krauss, G. J. Lamich, C. A. Melendres, M. H. Mendelsohn, M. J. Pellin, C. E. Young
Phone: (312)-972-3513

$1,022,000 03-3

Surface analysis by resonance ionization of sputtered atoms (SARISA) using pico-coulomb ion fluences combined with direct detection techniques; adsorbate structures, velocity and excited state distributions of sputtered species; mechanism of radiation-enhanced surface segregation in dilute alloy systems; synthesis of new shape-selective, catalysts incorporating small metal clusters; characterization and evaluation of catalysts using NMR, EPR, PAS, DTA, and Berty reactor techniques; electronic structure of matrix-isolated ligand-free transition metal clusters by laser fluorescence spectroscopy; electrocatalysis of O_2 reduction on metal-porphyrin and phthalocy-anine-coated electrode surfaces; dependence on pH of the viscosity and of the instantaneous and static shear moduli of biological surfactant monolayers.

LABORATORIES

BROOKHAVEN NATIONAL LABORATORY
Upton, Long Island, New York 11973

Metallurgy and Materials Science Division - 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
$290,000 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, R. C. Newman, N. Bandyopadhyay
Phone: (FTS) 666-4516 or (516)-282-4516
$400,000 01-2

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

072. SUPERCONDUCTING MATERIALS

D. O. Welch, M. Suenaga, J. Tafto, N. Higuchi
Phone: (FTS) 666-3517 or (516)-282-3517
$420,000 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.

LABORATORIES

BROOKHAVEN NATIONAL LABORATORY (continued)

073. PHYSICAL PROPERTIES OF METAL-INTERSTITIAL SYSTEMS

M. S. Pick (on leave), T. H. Metzger, 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. ELECTROCHEMICAL PROPERTIES OF INTERFACES

W. E. O'Grady
Phone: (FTS) 666-2829 or (516)-282-2829
$50,000 01-3

Studies of the role played by the structure, chemical composition, and oxidation states of the surface in electrode reactions using electrochemical techniques combined with low energy electron diffraction, Auger electron spectroscopy, X-ray photoelectron spectroscopy, and EXAFS.

075. PROPERTIES OF DEFECTS IN MATERIALS

C. L. Snead Jr.
Phone: (FTS) 666-3502 or (516)-282-3502
$300,000 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.

LABORATORIES

BROOKHAVEN NATIONAL LABORATORY (continued)

Department of Chemistry - 02 -

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

076. NEUTRON SCATTERING

L. M. Corliss, J. M. Hastings, R. Thomas
Phone: (FTS)-666-4376 or (516)-282-4376
$420,000 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.

Department of Physics - 02 -

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

077. MAGNETIC AND STRUCTURAL PHASE TRANSITIONS

S. M. Shapiro, J. D. Axe, D. P. Belanger, P. Böni, J. P. Wicksted, H. Yoshizawa
Phone: (FTS) 666-3822 or (516)-282-3822
$1,145,000 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.

078. ELEMENTARY EXCITATIONS AND NEW TECHNIQUES

G. Shirane, B. H. Grier, C. F. Majkrzak, L. Passell, S. K. Satija, O. Steinsvoll, J. P. Wicksted, Y. J. Uemura
Phone: (FTS) 666-3732 or (516)-282-3732
$1,490,000 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 polarizer and new devices for beam modulation.

LABORATORIES

BROOKHAVEN NATIONAL LABORATORY (continued)

079. X-RAY SCATTERING RESEARCH

D. E. Moncton, K. D'Amico, B. C. Frazer (on leave), L. D. Gibbs, H. Moudden
Phone: (FTS)-666-2741 or (516)-282-2741
$900,000 02-2

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

080. LOW ENERGY - PARTICLE INVESTIGATIONS OF SOLIDS

K. G. Lynn, D. Chen (CCNY), D. Fischer (SUNY-Stony Brook), W. Frieze, D. Gidley (Bell Labs), C. Lewis (DAS), B. Nielsen, L. Roelling (CCNY), C. L. Snead Jr. (DAS), M. Weber (CCNY)
Phone: (FTS) 666-3710 or (516)-282-3710
$955,000 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 interface and ion implanted and laser annealed semiconductors; use of recently developed SR channel at AGS.

081. ADVANCED MATERIALS SYNTHESIS AND CHARACTERIZATION

D. E. Cox, K. G. Lynn, A. Moodenbaugh
Phone: (FTS) 666-3818/3870 or (516)-282-3818/3870
$460,000 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.

LABORATORIES

BROOKHAVEN NATIONAL LABORATORY (continued)

082. 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
$660,000 02-3

Phase transitions, critical and cooperative phenomena in magnetic systems, organic metals and incommensurate structures; properties of one- and two-dimensional materials by analytic 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.

083. SURFACE PHYSICS RESEARCH

M. Strongin, S. Hulbert, P. D. Johnson, V. J. Murgai, S. Raeen, D. Wesner
Phone: (FTS) 666-3763 or (516)-282-3763
$850,000 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 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 NSLS. The problems presently being studied include: a) electronic properties of overlayers and clean metal surfaces, and hydrogen on metal surfaces. Besides valence band photoemission, inverse photoemission and core level spectroscopy are used as tools in this area; b) organic molecules on surfaces and properties of organic solids; c) surface metallurgy and surface compounds; d) cooperative effects and phase transitions in adsorbate layers on metal surfaces. 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.

LABORATORIES

BROOKHAVEN NATIONAL LABORATORY (continued)

High Flux Beam Reactor - 02 -

G. C. Kinne - Phone (FTS) 666-4061 or 516-282-4061
D. C. Rorer - Phone (FTS) 666-4056 or 516-282-4056

084. 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

$6,900,000 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.

LABORATORIES

BROOKHAVEN NATIONAL LABORATORY (continued)

National Synchrotron Light Source - 02 -

M. Blume: (FTS) 666-3735 or (516)-282-3735

085. NATIONAL SYNCHROTRON LIGHT SOURCE, OPERATIONS AND DEVELOPMENT
(see also page D-1)

M. Blume, M. Barton, K. Batchelor, R. Blumberg, J. Galayda, J. Godel, J. Hastings, H. Hsieh, R. Klaffky, S. Krinsky, A. Luccio, C. Pellegrini, W. Thomlinson, A. van Steenbergen, G. Williams
Phone: (FTS) 666-3735 or (516)-282-3735

$7,300,000 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 beam lines of the vacuum ultraviolet (VUV) and X-ray storage rings; and the technical support of experimental users. The development of the NSLS encompasses the further improvement of the storage rings to achieve maximum brightness photon sources and the further development of the photon lines of the facility by means of new developments in high resolution photon optics, state-of-the-art monochromators, X-ray mirror systems, detectors and other necesary 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 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.

LABORATORIES

IDAHO NATIONAL ENGINEERING LABORATORY
550 2nd Street
Idaho Falls, Idaho 84301

Materials Science Division - 01 -

D. D. Keiser - Phone (FTS) 583-1770 or (208) 526-1770

100. MATERIALS SCIENCE WELDING RESEARCH

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

$550,000 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. Heat source/molten pool interaction investigations utilizing high-speed cinematography, emission spectroscopy, laser-induced fluorescence spectroscopy, holographic interferometry, infrared thermography, and finite element (and difference) computer modeling. 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.

Vic Storhok 583-8135

Keefer - 8003

LABORATORIES

ILLINOIS, UNIVERSITY OF
at Urbana-Champaign
Urbana, Illinois 61801

333-1372

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

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 (see also page D-19)

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

$240,000 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

$165,000 01-1

Development of rapid solidification processing of alloys with powder preparation by laser, spin and centrifugal atomization and subsequent consolidation by dynamic compaction technqiues. 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

$150,000 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.

LABORATORIES

ILLINOIS, UNIVERSITY OF (continued)

109. GRAIN GROWTH IN ALUMINA

D. S. Phillips
Phone: (217)-333-6440

$70,000 01-1

Characterization of grain boundaries in solid-state and liquid-phase sintered aluminas by transmission electron and analytical electron microscopy. Correlation of boundary mobilities with microstructures.

110. PROCESSING AND CHARACTERIZATION OF NOVEL AMORPHOUS MATERIALS AND SURFACES

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

$55,000 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.

111. MICROCHEMISTRY OF SOLIDS

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

$65,000 01-1

Development of microanalytic methods for sulfur in coal. Studies of changes in pyrite, pyrrhotite and organic sulfur content during coal treatment and conversion.

112. PROCESSING AND MICROSTRUCTURE OF COMPLEX CERAMIC SYSTEMS

A. Zangvil
Phone: (217)-333-6829

$85,000 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.

113. HYDROGEN BEHAVIOR IN BCC METALS

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

$130,000 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.

LABORATORIES

ILLINOIS, UNIVERSITY OF (continued)

114. MICROMECHANICS AND MICROMECHANISMS OF FRACTURE

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

$270,000 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.

115. COUNCIL ON MATERIALS SCIENCE

D. Lazarus
Phone: (217)-333-0492

$75,000 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.

116. STRUCTURE, CRACKING AND CHEMISTRY OF CERAMIC GRAIN BOUNDARIES AND PHASE BOUNDARIES

S. D. Brown, A. Zangvil
Phone: (217)-333-4766 or (217)-333-6829

$65,000 01-2

Effects of impurities on structure and chemistry of regions contiguous to grain boundaries in SiC and Si_3N_4. Delayed failure, fracture toughness, creep and corrosion. Emphasis on effects of partial pressures of hydrogen on strength properties. Structure of AlN-SiC solid solutions.

117. PHYSICAL PROPERTIES OF CERAMIC MATERIALS

W. S. Williams
Phone: (217)-333-3524

$100,000 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.

LABORATORIES

ILLINOIS, UNIVERSITY OF (continued)

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

H. Chen ,
Phone: (217)-333-7636

$80,000 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.

119. DIELECTRIC SOLIDS

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

$120,000 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.

120. MICROSTRUCTURE AND CRYSTALLIZATION IN NOVEL GLASSY SYSTEMS

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

$90,000 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.

121. MICROWAVE STUDIES OF TUNNELING STATES IN DISORDERED MATERIALS

H. J. Stapleton
Phone: (217)-333-0073

$100,000 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.

LABORATORIES

ILLINOIS, UNIVERSITY OF (continued)

122. LOW TEMPERATURE STUDIES OF DEFECTS IN SOLIDS

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

$120,000 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 0.02-200K.

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

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

$150,000 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.

124. RESPONSE OF SOLIDS TO ELECTROMAGNETIC RADIATION

J. D. Dow
Phone: (217)-333-2981

$40,000 02-2

Theory of synchrotron radiation spectra of deep cores in metals and semiconductors. Theory of semiconductor surface states. Theory of surface reconstruction geometries of semiconductors. Theory of disordered systems and alloys.

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

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

$170,000 02-2

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.

LABORATORIES

ILLINOIS, UNIVERSITY OF (continued)

126. EXCITON COLLECTION FROM ANTENNA SYSTEMS INTO ACCESSIBLE TRAPS

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

$10,000 02-2

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.

127. HIGH-FIELD SUPERCONDUCTORS

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

$70,000 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.

128. ULTRASONIC STUDIES OF THE STRUCTURE OF MATTER

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

$150,000 02-2

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

129. DEFECT AND ELECTRONIC PROPERTIES OF SOLIDS

D. Lazarus
Phone: (217)-333-0492

$25,000 02-2

Atomic mobility and electrical conduction in solid electrolytes and metallic glasses, studied as a function of temperature and pressure. Mainly concerned with elucidating atomistic defect formation and jump processes.

LABORATORIES

ILLINOIS, UNIVERSITY OF (continued)

130. PROPERTIES OF CRYSTALLINE CONDENSED GASES

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

$190,000 02-2

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

131. NUCLEAR MAGNETIC RESONANCE IN SOLIDS

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

$170,000 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.

132. PHYSICAL PROPERTIES OF ORDERED AND DISORDERED SOLID SOLUTIONS

H. Zabel
Phone: (217)-333-2514

$150,000 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.

LABORATORIES

LAWRENCE BERKELEY LABORATORY
University of California
Berkeley, California 94720

Materials and Molecular Research Division

A. W. Searcy - Phone: (415) 486-6062 or FTS: 451-6062

140. STRUCTURE AND PROPERTIES OF TRANSFORMATION INTERFACES

R. Gronsky
Phone: (FTS) 451-5674 or (415)-486-5674
$170,000 01-1

Transformation interfaces include homophase boundaries, heterophase boundaries and "free" surfaces at which solid state reactions are either initiated or propagated. The atomic configurations of such interfaces and the establishment of the relationship between their structure and relevant interfacial properties. Correlations between the segregation behavior, precipitation behavior and deformation behavior of interfaces and their detailed defect structures. Experiments are chiefly by transmission electron microscopy, including energy dispersive X-ray and electron energy loss spectroscopies; results are correlated with theoretical predictions of interfacial phenomena.

141. DESIGN, MICROSTRUCTURE, AND PROPERTIES OF ALLOYS: INORGANIC MATERIALS

G. Thomas
Phone: (FTS) 451-5656 or (415)-486-5656
$580,000 01-1

A multicomponent, interdisciplinary program in physical metallurgy and ceramics involving fundamental quantitative studies of the structure-property relationships in technologically significant materials involved in energy and conservation. Characterization of both structure and composition at the highest levels of spatial (transmission electron microscopy) and chemical (spectroscopy) resolutions. Specific tasks include: a.) dual phase, ferrite-martensite steels for rod and wire, optimization of microstructure and processing, analytical studies of solute partitioning, fatigue, and wear; b.) martensitic and bainitic steels, fundamental studies of phase transitions, relation to wear; surface treatments (laser technology), grain boundary precipitation, effect of copper; c.) magnetic materials; structure of audio recording tape, piezoelectric materials, rare-earth alloys.

LABORATORIES

LAWRENCE BERKELEY LABORATORY (continued)

142. SOLID STATE PHASE TRANSFORMATION MECHANISMS

K. H. Westmacott
Phone: (FTS) 451-5663 or (415)-486-5663
$190,000 01-1

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

143. NATIONAL CENTER FOR ELECTRON MICROSCOPY (see also page D-28)

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
$1,090,000 01-1

Organization and operation of a national, user-oriented resource for transmissision 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 Microscopy (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
$105,000 01-1

Kinetics of reactions between gases and solids; the role of microstructure. Relations between the sites for nucleation and growth of second phases and microstructural features such as microcracks, grain boundaries and dislocations. Environmental cell experiments in the high voltage transmission microscope.

LABORATORIES

LAWRENCE BERKELEY LABORATORY (continued)

145. LOCAL ATOMIC CONFIGURATIONS IN SOLID SOLUTIONS

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

$105,000 01-1

Fundamental investigation of ordering and phase separation in certain metallic alloys. Both theoretical and experimental aspects for the three following topics: atomic ordering in systems exhibiting the phenomenon of long-period superstructure formation; the theoretical tool being primarily the newly developed cluster variation method of statistical thermodynamics; the experimental tool being high-resolution electron microscopy. Phase separation in systems exhibiting partitioning of substitutional and interstitial alloying elements, such as alloy steels; the theoretical tool here being multicomponent nucleation theory and the experimental one being transmission electron microscopy with full analytical capabilities. The interaction of magnetic and ionic ordering in AuFe alloys which exhibit the spin glass phenomenon; the theoretical tool is a modification of the cluster variation method, the experimental one that of high-resolution transmission electron microscopy and diffraction.

146. COLLABORATIVE RESEARCH BY TRANSMISSION ELECTRON MICROSCOPY

A. W. Searcy
Phone: (FTS)451-6062 or (415)-486-6062

$50,000 01-1

This program has been established 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. Under the program, postdoctoral, or more mature visiting electron microscopists spend up to one year at LBL using the unique instrumentation available at the National Center for Electron Microscopy in (NCEM) collaborative programs with Materials and Molecular Research Division Investigators recommended for support by the NCEM Steering Committee.

LABORATORIES

LAWRENCE BERKELEY LABORATORY (continued)

147. THEORETICAL PROBLEMS IN ALLOY DESIGN

J. William Morris Jr.
Phone: (FTS) 451-6482 or (415)-486-6482; (415)-642-3815

$540,000 01-2

A multifaceted program of metallurgical research on the science of alloy design. Specific research tasks include: (1) theoretical research on phase transformations in solids and on the influence of microstructure on engineering properties; (2) experimental research on fundamental problems in metallurgy, including the control of microstructure through thermomechanical processing, the influence of microstructure on engineering properties, and the development of probative materials testing techniques; (3) the development of new structural alloys for advanced energy systems, a task mainly concerned with the design of improved structural alloys for low-temperature use; (4) welding metallurgy, including the development of appropriate weld filler metals and weld microstructures to maintain toughness in high strength welded alloys; (5) the development of improved superconducting wires for use in high field superconducting magnets.

148. MECHANICAL PROPERTIES OF CERAMICS

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

$305,000 01-2

The development of predictive capabilities for the high temperature failure of ceramics and for microstructure/defect development during sintering. Elevated temperature failure studies are concerned with the initiation, growth and coalescence of cracks during creep. Experimental measurements are being correlated with theoretical models containing the dominant microstructural variables. Sintering studies are examining the processes that dictate the presence of retained porosity and defects during solid state and liquid phase sintering.

LABORATORIES

LAWRENCE BERKELEY LABORATORY (continued)

149. ENVIRONMENTALLY AFFECTED CRACK GROWTH IN ENGINEERING MATERIALS

R. O. Ritchie
Phone: (FTS) 451-5798 or (415)-486-5798; (415)-642-0417

$240,000 01-2

A program to examine the respective roles of mechanical, micromonotonic and cyclic growth of flaws in engineering materials. Current emphasis is being devoted: i) to defining the role of environment and microstructure on microscopic crack closure mechanisms and their effect on subsequent near-threshold fatigue growth of long and short cracks in steels below 10^{-5} mm/cycle, for inert, gaseous, aqueous and viscous environments; ii) to the modelling of crack growth toughness. Characterization of macroscopic growth rate behavior and microscopic failure mechanisms using fracture mechanics, microstructural and surface chemistry (e.g., Auger and ESCA) analysis and detailed fractography.

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) 451-6062 or (415)-486-6062

$295,000 01-3

Emphasis on endothermic decomposition reactions. A general theoretical analysis of decomposition reaction kinetics; a systematic investigation of the separate influences of temperature, product gas pressure, thermal energy balance, particle size, sample size, and catalysts on decomposition rates and on the structure and properties of solid-reaction products; TEM studies of prototype decomposition reactions. Vapor transport through porous solids to obtain quantitative data on high-temperature surface diffusion; theoretical and experimental studies of surface thermodynamics, chemisorption and surface-transport processes.

LABORATORIES

LAWRENCE BERKELEY LABORATORY (continued)

152. STRUCTURE-PROPERTY RELATIONSHIPS IN SEMICONDUCTOR MATERIALS

J. Washburn
Phone: (FTS) 451-6254 or (415)-486-6254
$330,000 01-3

A research program is to advance the understanding of structural defects including the structure of interfaces in semiconductor materials. Particular emphasis on interfaces and defects that are formed during processing steps used for state-of-the-art, solid-state-device manufacture such as ion implantation, oxidation, and contact formation. Studies of the crystalline-to-amorphous transformation during ion damage in silicon and gallium arsenide; an investigation of the detailed mechanisms of crystal growth into amorphous zones; and a study of the growth of Cu_2S layers on the surface of CdS. High-resolution lattice-imaging electron microscopy combined with computer simulation of the images to reveal and interpret fine-scale defects and interface structures, in conjunction with complementary observations such as Rutherford backscattering measurements, secondary ion mass spectroscopy, and electrical or optical 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

Studies of the reactions at ceramic/metal interfaces and their effect on the physical properties of such interfaces. Two different reaction types are considered: Gaseous reduction of transition metal oxides; and subscale oxidation of Ni/ZrO_2 interfaces. Thermogravimetrical analysis, and electron microscope methods to characterize the reaction mechanisms. Acoustic emission detection during thermal cycling to assess the integrity of the metal/ceramic joint. Reactions in the solid state during densification in the $CaO-Al_2O_3$ system.

154. STRUCTURE AND ELECTRICAL PROPERTIES OF COMPOSITE MATERIALS

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

The relationship of the properties of hard carbons and soft carbons to their structure. Glassy carbon studied as a model hard carbon. Specific atomic mechanism(s) associated with the structural changes during graphitization.

LABORATORIES

LAWRENCE BERKELEY LABORATORY (continued)

155. HIGH-TEMPERATURE OXIDATION AND CORROSION OF MATERIALS

A. W. Searcy
Phone: (FTS) 451-6062 or (415)-486-6062

$350,000 01-3

A program to understand: a) the mechanisms by which materials withstand high-temperature corrosive attack, and b) 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 scales structure, morphology, and growth mode; the chemical integrity of the scale when exposed to corrosive sulfate deposits. The ultimate goal is to relate mechanisms of behavior to the thermodynamic, diffusional, structural, and compositional parameters of the metal oxides, sulfides, and other phases involved, and to develop both quantitative and predictive alloy corrosion models.

156. CERAMIC INTERFACES

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

$125,000 01-3

Development of an improved understanding of processes that control microstructural changes during materials fabrication and utilization. Thermodynamic and kinetic models of the modifying effect of dihedral angle on the morphological stability of continuous grain boundary phases, e.g., continuous pore channels present during sintering and continuous second phases in eutectic alloys and composites. The effect of solute additions, specifically MgO, on the nature of grain boundary migration in pore-free Al_2O_3. Grain boundary migration in lead. Fabrication of oxide powders to study particle coarsening by vapor phase transport. The recrystallization behavior of cold-pressed, NaCl powder.

157. ABRASIVE, EROSIVE AND SLIDING WEAR OF MATERIALS

I. Finnie
Phone: (415)-642-1496

$120,000 01-5

Determination of the-basic mechanisms of abrasive, erosive and sliding wear. Identification of similarities and differences in different types of wear to allow development of simpler screening tests. Examination of material properties and microstructural features needed for optimum wear resistance. Development of quantitative methods of wear prediction for both single phase and heterogeneous materials.

LABORATORIES

LAWRENCE BERKELEY LABORATORY (continued)

158. EROSION-CORROSION WEAR PROGRAM

A. W. Searcy
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 erosion and strength degradation of brittle coatings and layers subject to impact by solid particles. Studies of the damage created by individual particles and of the erosion characteristics under multiple impact conditions; consideration of residual stresses in the coatings and the adherence to the substrate. Predictions of material removal by spalling, after projectile impact.

160. FAR INFRARED SPECTROSCOPY

P. L. Richards
Phone: (415)-642-3207

$228,000 02-2

Development of improved types of infrared detectors, mixers, and spectrometers. Improved infrared techniques for experiments in areas of fundamental and applied infrared physics. Developments of infrared technology: a liquid helium cooled diffraction grating spectroscopy, fabrication and testing of ultrasensitive photoconductive detectors for the 50-500 μm wavelength range, improved fabrication for bolometric detectors with improved ultimate sensitivity, development of a new class of far infrared dichroic beam dividers, and development of far infrared harmonic generation as a spectroscopic source. Experiments in progress: measurements of the near infrared absorption spectra of molecules chemically adsorbed on metal surfaces, measurements of the infrared spectra of one-dimensional conductors including charge-density wave systems and organic superconductors, and measurements of the infrared photoconductivity of impurities in semiconductors.

LABORATORIES

LAWRENCE BERKELEY LABORATORY (continued)

161. EXPERIMENTAL SOLID STATE PHYSICS AND QUANTUM ELECTRONICS

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

$264,000 02-2

Emphasis is on development of linear and nonlinear laser and optical techniques for material studies and applications of these techniques to study linear and nonlinear optical properties of gases, liquids, liquid crystals, and solids. Both theoretical and experimental research on various aspects of light interaction with matter. Newly developed techniques used to study current problems of interest: isotope separation, photochemistry, surface physics, and phase transitions, and other nonlinear optical effects in matter.

162. EXCITATION IN SOLIDS

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

$170,000 02-2

Studies of the onset of instabilities and pseudorandum behavior in solids, detailed analysis and interpretation within the recently developed renormalization group theory of chaotic dynamics, which displays universality and predicts that similar and recognizable modes of behavior will be observed in a very broad class of nonlinear phenomena, e.g., turbulence in fluids; plasma instabilities; erratic behavior in nonlinear mechanical, electrical and chemical systems; and various instabilities in semiconducting, magnetic, ferroelectric and piezoelectric materials. To facilitate direct comparison between observed behavior and theoretical models, development of specific experimental methods: bifurcation diagrams, phase space portraits, Poincare sections, return maps, power spectral analysis, real time and transient analysis, and probability density distributions. Concentration on spin waves in ferrities and on semiconductors. A detailed and systematic study of the chaotic dynamics of driven p-n junctions in Si and Ge revealed many universal patterns: periodic doubling bifurcations, onset of chaos, periodic windows, and intermittency. Spin wave instabilities in ferrite spheres display period doubling, chaos, and intermittency and understood by two-dimensional quadratic map. Electron-hole plasma density waves in crystals of Ge exhibit a period doubling route to chaos, periodic windows, and quasi-periodicity. Results bear on devices of high technological interest, and on a very general class of nonlinear problems of practical importance.

LABORATORIES

LAWRENCE BERKELEY LABORATORY (continued)

163. TIME RESOLVED SPECTROSCOPIES IN SOLIDS

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

$80,000 02-2

Use of fast picosecond tunable laser pulses produced by modelocked dye lasers, to study the processes associated with interactions between elementary excitations in condensed matter in real time to determine strength of these interactions. Current investigations involve: properties of dense electron-hole plasma created by picosecond laser pulses in semiconductors by light scattering spectroscopies and time-resolved emission spectroscopy; trapping of free carriers at deep, nonradiative centers in crystalline or disordered semiconductors; and carrier relaxation mechanisms in crystalline and amorphous solids.

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

J. Clarke
Phone: (415)-642-3069

$288,000 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, nonequilibrium superconductivity, and the measurement of electrical noise. An ultra low noise SQUID amplifier operating at frequencies of up to 100 MHz used to improve the sensitivity of nuclear magnetic resonance and 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 investigations of macroscopic quantum tunneling in Josephson tunnel junctions at millikelvin temperatures. The nonlinear dynamics of circuits containing a Josephson junction being studied, with particular regard to the noise in such systems. A detailed study of the excess noise induced in metal films by electron bombardment in an electron microscope. This type of measurement may provide a new technique for characterizing the defect concentration of metals.

LABORATORIES

LAWRENCE BERKELEY LABORTORY (continued)

165. THEORETICAL STUDIES OF THE ELECTRONIC PROPERTIES OF SOLID SURFACES

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

$75,000 02-3

A study of the properties of solid surfaces, in particular: (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 temperature; (c) Electronic structure of surfaces, electron states and electron densities in the neighborhood of the surface; (d) Vibronic properties of surfaces; (e) Magnetic properties of surface, both in magnetic solids (ferromagnetic and antiferromagnetic) or in nonmagnetic solids which may develop a magnetic surface layer; (f) Chemical catalytic properties of solids as they are related to basic physical properties (a)-(e). A variety of theoretical techniques and models to focus on the various properties (band-structure models, many-body body electron physics, numerical relaxation techniques) developed, but the emphasis is on physical aspects and their implication to experiments rather than techniques per se.

166. THEORETICAL SOLID STATE PHYSICS

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

$105,000 02-3

To provide a microscopic theory of solids capable of explaining and predicting the physical properties of real materials. A successful theory based on a quantum mechanical pseudopotential-local density-total energy approach with inputs essentially of only the atomic number and atomic mass of the constituent atoms making up a solid developed. Applications of the method to: surfaces, interfaces, optical properties, superconductivity, electronic structure, vibrational properties, static structural properties, high pressure solid phase transitions, transport, photoemission, chemisorption, and properties of molecules. Direct collaborations with experimental projects are frequent, and the predictive power of the approach has been tested successfully.

LABORATORIES

LAWRENCE BERKELEY LABORATORY (continued)

167. LOW TEMPERATURE PROPERTIES OF MATERIALS

N. E. Phillips
Phone: (415)-642-4855

$130,000 03-1

Research on low temperature properties of materials and on methods of temperature measurement. Measurements on ^{3}He in the Fermi-liquid region have established the correct values of parameters which 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 CuMn in high magnetic fields that have mapped out the theoretically predicted phase boundary of the spin-glass phase. Specific future objectives: an extension of the ^{3}He measurements to the superfluid phases, additional studies on spin glasses, and specific heat measurements at pressures to 20 kbar on mixed-valence compounds.

168. ELECTROCHEMICAL PROCESSES

C. W. Tobias
Phone: (415)-642-3764

$120,000 03-1

Novel methods for reducing mass transfer resistance in high rate applications, e.g. effects of fixed flow obstacles and of suspended inert solid particles in flowing electrolytes. Nonaqueous ionizing solvents investigated for potential use in ambient temperature electrosynthesis processes. Techniques for the removal of trace impurities in propylene carbonate to below 10 ppb., to improve solvent stability in presence of energetic oxidizing- or reducing-agents.

169. HIGH-TEMPERATURE THERMODYNAMICS

L. Brewer
Phone: (415)-486-5946

$160,000 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.

LABORATORIES

LAWRENCE BERKELEY LABORATORY (continued)

170. CHEMISTRY AND MATERIALS PROBLEMS IN ENERGY PRODUCTION TECHNOLOGIES

D. R. Olander
Phone: (415)-642-7055

$275,000 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.

171. PLASMA ENHANCED DEPOSITION OF THIN FILMS

D. W. Hess
Phone: (415)-642-4862

$20,000 03-3

Research on rf plasma enhanced deposition of thin films. Control of chemical, physical, and electrical properties by variation of deposition parameters. The final phase of this program.

LABORATORIES

LAWRENCE BERKELEY LABORATORY (continued)

172. ELECTROCHEMICAL PHASE BOUNDARIES

R. H. Muller
Phone: (FTS) 451-6079 or (415)-486-6079
$180,000 03-3

To advance the understanding of boundary layers and thin films at electrochemical interfaces. New optical techniques for the observation of electrode surfaces in liquid media developed and used: spectroscopic ellipsometry combined with light scattering measurement, Auger spectroscopy, interferometry, thin film interference, and Doppler velocimetry.

173. SOLID STATE AND SURFACE REACTIONS

G. A. Somorjai
Phone: (FTS) 451-6160 or (415)-486-6160; (415)-642-4053
$390,000 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; (415)-642-1220
$195,000 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.

LABORATORIES

LAWRENCE BERKELEY LABORATORY (continued)

Accelerator and Fusion Research Division - 02 -

175. R&D ON ADVANCED PHOTON SYSTEM

T. Elioff, R. Yourd, D. Attwood
Phone: (FTS) 451-4024 or (415)-485-4024
$2,200,000 02-2

Research and development of advanced accelerator systems and state-of-the-art components for high-brightness synchrotron beamlines and advanced insertion devices (wigglers and undulators). Associated research activities include the development of next-generation wigglers and undulators, of advanced beam line components and optical elements. Experimental facilities developed to match the needs of future experiments requiring high spectral brilliance. Accelerator Research includes the development of advanced computer control systems, precision instrumentation, radiofrequency systems with reduced higher order modes, a fast booster extraction system, ultra high vacuum systems and techniques, and studies to assure attainment of high current-low emittance electron beams for maximum spectral brilliance.

176. CENTER FOR X-RAY OPTICS (see also page D-27)

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

LABORATORIES

LAWRENCE BERKELEY LABORATORY (continued)

177. CENTER FOR ADVANCED MATERIALS: CATALYSTS CERAMICS; ELECTRONIC MATERIALS; POLYMERS; INSTRUMENTATION FOR SURFACE SCIENCE

K. S. Pitzer, J. Clarke, L. C. De Jonghe, M. M. Denn, E. E. Haller, G. A. Somorjai, A. G. Evans
Phone: (FTS) 451-4755 or (415)-486-4755

$2,300,000 01-1, 02-2, 03-3

Investigations of the mechanisms of defect formation and contamination during bulk crystal growth of gallium arsenide and other III-V semiconductors. Investigations of the relationship between the structure and electronic properties of semiconductor interfaces, and determination of the effects of substrate defects on the quality of epitaxial thin films. Synthesis and structural and catalytic characterization of heterogeneous catalysts: zeolites, transition metal compounds, and other novel catalytic materials. Investigations of the relationship between processing and microstructures of structural polymers and polymer composites focusing on polymer liquid crystals, short-fiber polymer composites, block copolymers, coprocessing of immiscible fluids, and interactions among polymers, solvents, and non-solvents. Development of advanced instrumentation (such as a tunneling microscope) for characterizing surfaces and interfaces that are important to high-technology or materials-based industries. Investigations to strengthen the scientific base needed for the development of advanced, high-temperature structural ceramics. Areas of study here include colloid behavior of powders, ceramic fabrication, high temperature mechanical properties of ceramics and evaluation of erosion and wear. Research on powder suspensions, sintering, crack nucleation and failure prediction is included.

LABORATORIES

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

Chemistry & Materials Science Department

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: (FTS) 543-2653 or (415)-443-2653

$420,000 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 LASER, ELECTRON AND ION BEAMS

E. N. Kaufmann
Phone: (FTS) 543-2640 or (415)-423-2640

$230,000 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.

LABORATORIES

LAWRENCE LIVERMORE NATIONAL LABORATORY (continued)

192. RAPID SOLIDIFICATION, COMPACTION, AND STRUCTURAL CHANGES BY DYNAMIC PRESSURE

W. J. Nellis, W. C. Moss, H. B. Radousky
Phone: (FTS) 532-7200 or (415)-432-7200
$100,000 01-1

Structures of materials induced by high dynamic pressure of $\lesssim$1 Mbar. Cause and effect relationship between the initial and final material states and the dynamic path that connects them. Structure and residual effects of dynamic pressure on the superconducting transition temperature of Nb and the magnetic properties of Fe. Variation of microstructure of anisotropic magnetic compounds by rapid quenching from high dynamic pressure, density and temperature and the effect on material strength and magnetization.

193. OPTICAL MATERIALS RESEARCH

N. Winter
Phone: (FTS) 532-6215 or (415)-422-6215
$470,000 02-2

New optical materials for high-power lasers prepared and characterized. Materials of interest include both transmitting optics and active media for solid-state lasers. Optical spectroscopy used to determine those properties affecting the energy storage and extraction capabilities of different laser ion-host combinations. Nonlinear optical properties of materials subject to intense light beams are also investigated. Studies of multiphoton absorption processes and intensity-dependent changes in refractive index. Measurements of optical and spectroscopic properties correlated with theoreticl calculations of local fields and electronic structure. State-of-the-art theoretical calculations of the optical properties of various ion-host combinations. The growth of new oxide and fluoride crystals for laser and nonlinear optics applications explored and measurements made of their physical and chemical properties.

194. SURFACE PHYSICS AND CHEMISTRY OF LASER-INDUCED DAMAGE

W. J. Siekhaus
Phone: (FTS) 532-6884 or (415)-432-6884
$300,000 02-2

Investigation of physical and chemical mechanisms leading to laser surface systems. Experiments measuring with high spatial resolution multiphoton electron emission from semiconductor and insulator surfaces. Spacially resolved time of flight mass spectrometric studies of laser induced ion emission resulting in laser surface damage.

Don Sandstrom L X4553
Milt Haas X2338

LABORATORIES

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

Materials Science and Technology Division - 01, 03

S. S. Hecker - Phone (FTS) 843-4563 or 505-667-4563

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, N. F. Kochs, P. Follansbee, P. Martin
Phone: (505)-667-6750

$590,000 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. Multi-axial loading brittle fracture responses of Al_2O_3, Si_3N_4, SiC and ZrO_2; Statistical fracture theories for mixed-mode fracture of indention-produced surface flaws and macroscopic cracks; microstructural effects on multiaxial loading brittle fracture.

LABORATORIES

LOS ALAMOS NATIONAL LABORATORY (continued)

202. STRUCTURAL CERAMICS

J. J. Petrovic, D. S. Phillips
Phone: (505)-667-5913

$290,000 01-5

Fabrication-microstructure-properties interrelationships for structural ceramic materials; synthesis of dense, strong SiC and Si_3N_4 without the use of densification additives that can degrade elevated temperature mechanical properties and affect property reproducibility; RF-plasma synthesis of ultra-fine/ultra-pure SiC and Si_3N_4 powders; powder activation to enhance densification, using explosive shock loading and ion irradiation treatments; colloidal chemistry approaches to the synthesis of high green density bodies with uniform porosity distribution; dependencies of properties on processing and microstructure.

203. IMPURITY MODIFICATION OF MATERIALS: SURFACE PROPERTIES AND THIN STRUCTURAL FILMS

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

$240,000 03-2

Selective modification of chemisorption properties by surface additives. Relationship that electronic, structural, and compositional factors have to surface reactivity. Study of vapor deposited metal and semimetal adatoms on single-crystal desorption spectroscopies, low-energy electron diffraction and work function measurements. Crystallographic characterization by MeV ion scattering. Structural and mechanical properties of vapor deposited thin film metal/metal-compound laminates. Spatial and chemical nature of impurity layers by energetic ion beam analysis and conventional surface sensitive techniques. Physical and mechanical properties of vapor deposited films.

LABORATORIES

LOS ALAMOS NATIONAL LABORATORY (continued)

Physics Division - 02 -

J. C. Browne - Phone (FTS) 843-6162 or 505-667-6162

204. CONDENSED MATTER RESEARCH WITH THE SNR/PSR FACILITY (see also page D-9)

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

$1,570,000 02-1

Neutron scattering research in condensed matter using the SNR/PSR pulsed spallation neutron source at Los Alamos. Studies in most areas of condensed matter; currently metal hydrides, catalysts, liquids, metallic glasses, magnetism, chemical structure, chemical spectroscopy, etc. The SNR/PSR is a national user facility for neutron scattering research in solid state physics, chemistry, materials science, biology, and polymers with the following time-of-flight spectrometers currently in the user program: single-crystal diffractometer, filter difference spectrometer and a powder diffractometer.

205. ULTRAHIGH-PRESSURE STUDIES OF MOLECULAR CRYSTALS

R. L. Mills
Phone: (505)-667-4129

$220,000 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.

206. THERMAL PHYSICS

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

$250,000 02-2

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 is superfluid ^{4}He near 1 K, steady and oscillatory, nonlinear dynamics, coherence and chaos; spin polarized hydrogen isotopes: transport, thermodynamic properties, magnetosound; normal and superfluid liquid ^{3}He: ferromagnetism, susceptibility anisotropy.

LABORATORIES

LOS ALAMOS NATIONAL LABORATORY (continued)

Theoretical Division - 01, 02

G. I. Bell - Phone: (FTS) 843-4401 or 505-667-4401

207. ELASTIC WAVE SCATTERING AND QUANTITATIVE FLAW AND MICROSTRUCTURE CHARACTERIZATION

J. E. Gubernatis
Phone: (505)-667-6727

$180,000 01-5

Development of an analytical scientific reference data base for flaw and microstructure characterization calculations of phenomena selected as representative of applications; integral equation methods, the method of optimized truncation, geometrical diffraction theory and Pade approximations; single scattering results for the flaw characterization studies; multiple scattering theories for the microstructure characterization studies. Investigate use of elastic wave scattering measurements for residual stress evaluation and for characterization of surface cracks.

208. LOS ALAMOS EQUATION OF STATE LIBRARY

J. D. Johnson
Phone: (505)-667-4053

$250,000 02-3

A computer-based library of equations of state (EOS) and other material properties such as opacities, and electrical and thermal conductivities for application to energy and related programs. Survey current user requirements and calculate or acquire and evaluate the needed data Data in tabular form suitable for use in realistic hydrodynamic code calculations and other applications. Library programs and data available to users on magnetic tapes in a universal computer format. Theories of solids, liquids, gases, plasmas, and mixtures used to generation of EOS data. Development of new theoretical methods when existing theories and experiments are insufficient to satisfy user requirements.

LABORATORIES

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

Metals and Ceramics Division - 01 -

J. R. Weir, Jr. - Phone (FTS) 624-4065 or 615-574-4065
C. J. McHargue - Phone (FTS) 624-4344 or 615-574-4344

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

$632,000 01-1

The KKR-CPA method for calculating the electronic states of alloys provides the basis for explaining experiments on alloy systems such as photoemission, positron annihilation, soft X-ray emission and absorption, resistivity, low-temperature specific heats, etc. The high-speed band theory technique QKKR is used to calculate total energies of metals and intermetallic compounds. Results are coupled with KKR-CPA calculations to obtain insights into the thermodynamic parameters that determine the phase stability of alloy systems. The KKR-CPA method is used to study magnetism at finite temperatures, and order in alloys. Electron-phonon interactions are calculated and used to explain resistivities of normal metals and superconductors. Cluster and layer techniques are used to calculate the physical and chemical properties of surfaces interacting with their environment. Studies of metal-metalloid clusters are applied to grain-boundary segregation and cohesion.

216. X-RAY RESEARCH USING SYNCHROTRON RADIATION

C. J. Sparks, B. S. Borie, G. E. Ice, H. L. Yakel
Phone: (615)-574-6996

$639,000 01-1

Development and use of flourescence, anomalous dispersion, and scattering techniques for X-rays at the Stanford Synchrotron Radiation Laboratory; design and construction of beam line for installation at the National Synchrotron Light Source, Brookhaven National Laboratory; long- and/or short-range order in Fe-Ni-Cr alloys; atom positions in sigma phase, and alloyed carbides; defects in ion implanted materials; theoretical studies of extinction phenomena.

LABORATORIES

OAK RIDGE NATIONAL LABORATORY (continued)

217. MICROSCOPY AND MICROANALYSIS

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

$432,000 01-1

Development and application of analytical transmission microscopy and HVEM to determine the microstructure and microchemistry of solids; weakbeam darkfield studies of precipitates in irradiated alloys; lattice imaging of two-phase interfaces; SAES and EELS of internally oxidized refractory metal alloys; structure of long-range ordered alloys; in situ deformation, oxidation, and hydriding studies in the 1-MeV microscope; grain boundary phases in structrural ceramics; structure of metallic glasses; standardless EELS analysis; development of Imaging Atom Probe.

218. DEFORMATION AND FRACTURE OF METALS AND ALLOYS

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

$498,000 01-2

Experimental and theoretical studies of effects of impurities and interfaces on deformation and fracture of Ni, Fe-Ni, Ni-Cr, Fe-Ni-Cr, and Ni_3Al alloys; grain boundary cavity nucleation and growth; segregation of impurities to grain boundaries and creep cativities; dynamic recrystallization; small-angle neutron scattering studies of cavity growth during creep and fatigue in nickel and austenitic stainless steel.

219. MECHANICAL PROPERTIES OF CERAMICS

P. F. Becher, M. K. Ferber, C. S. Yust, P. Angelini
Phone: (615)-574-5157

$539,000 01-2

Toughening behavior and slow crack growth mechanisms in polycrystalline TiB_2 as related to internal stress, microcracking, and microstructure; wear studies of TiB_2, SiC, Al_2O_3, and transformation-toughened Al_2O_3-Zr_2O_3; slow crack growth and toughening behavior in transformation-toughened Al_2O_3-Zr_2O_3, dispersion-toughened SiC.

220. KINETICS AND MECHANISMS OF SURFACE AND SOLID STATE REACTIONS

J. V. Cathcart, R. E. Druschel, R. A. McKee, R. E. Pawel
Phone: (615)-574-4925

$533,000 01-3

Reaction kinetics and defect interactions during diffusion in growing sulfide scales; high temperature oxidation of Ni_3Al-base alloys; diffusion in doped FeS crystals; oxide scale adherence studies; dynamic resonance measurements of elastic and anelastic properties of scales; theoretical treatment of diffusion in highly defective oxides.

LABORATORIES

OAK RIDGE NATIONAL LABORATORY (continued)

221. METASTABLE MATERIALS

D. M. Kroeger, D. S. Easton, J. A. Horton
Phone: (615)-574-5156

$530,000 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 separation in metallic glasses.

222. RADIATION EFFECTS

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

$1,540,000 01-4

Mechanisms of radiation effects; neutron damage in pure metals, alloys, and ceramics irradiated in ORR, HFIR, and EBR-II, 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.

223. FUNDAMENTALS OF WELDING AND JOINING

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

$444,000 01-5

Control of weld microstructure through control of solidification parameters; composition, distribution, and stability of microphases; microstructure of laser-produced welds; hot cracking; modeling of solidification processes; structure-property correlations, austenitic and ferritic stainless steels, electron beam welding, American Welding Technology Application Center (AWTAC) Projects.

LABORATORIES

OAK RIDGE NATIONAL LABORATORY (continued)

224. HIGH TEMPERATURE ALLOY DESIGN

C. T. Liu, J. A. Horton, A. DasGupta, W. C. Oliver
Phone: (615)-574-4459

$344,000 01-5

Design of ductile polycrystal alloys based on Ni_3Al; microalloying with B; macroalloying with Fe, Hf, Ce; creep, oxidation and physical properties; structure and composition of grain boundaries, nature and effects of defects.

225. RESEARCH IN CERAMIC PROCESSING

P. F. Becher, C. B. Finch, P. Angelini, A. Bleier, S. Baik
Phone: (615)-574-5157

$399,000 01-5

Sintering behavior of TiB_2 including liquid phase effects, the role of oxygen and carbon; AEM characterization of second phase formation, crystal growth and characterization of properties of boride phases; synthesis of ZrO_2 and Al_2O_3 powders and effects of powder surface characteristics on densification in transformation-toughened Al_2O_3-ZrO_2 type composites; AEM studies on alloying and microstructural effects in transformation behavior.

226. ION BEAM PROCESSING OF MATERIALS

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

$250,000 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).

LABORATORIES

OAK RIDGE NATIONAL LABORATORY (continued)

Solid State Division - 02 -

M. K. Wilkinson - Phone (FTS) 624-6151 or 615-574-6151
F. W. Young, Jr. - Phone (FTS) 624-5501 or 615-574-5501

227. INTERATOMIC INTERACTIONS IN CONDENSED SYSTEMS

R. M. Nicklow, J. R. Arthur, J. W. Cable, H. R. Child, S. Funahashi, J. B. Hayter, S. Kawarazaki, W. C. Koehler, J. W. Lynn, H. A. Mook, R. M. Moon, O. A. Pringle, H. G. Smith, Y. Tsunoda
Phone: (615)-574-5240

$1,080,000 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 α-Ce, SmB_6, Ba, and intercalated graphite; magnetic excitations in Cu(Mn), amorphous materials, paramagnetic Ni and Fe, and Gd; phase transitions in In(Tl) alloys, Ni_3Mn, Cu_3Au, and random field systems; magnetic form factors of mixed-valence materials; structures of composition modulated systems and nuclear spin ordering.

228. PROPERTIES OF DEFECTS, SUPERCONDUCTORS, AND HYDRIDES

J. W. Cable, J. R. Arthur, H. R. Child, S. Funahashi, M. Iizumi, S. Katano, W. C. Koehler, H. A. Mook, R. M. Moon, 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 A15 com-pounds, $PdTe_2$, Fe(Cr) alloys, and KCl(CN); proton diffusion in biological systems and microemulsions; magnetic structures in GdD_2 and reentrant superconductors; SANS from coal solutions, oil shale, surfactants, metal alloys, and polymer blends; kinetics of spinodal decomposition.

229. SUPPORT FOR NEUTRON USERS' PROGRAM (see also page D-5)

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

$320,000 02-1

ORNL neutron scattering facilities available to outside scientists through Neutron Users' Program; recent investigations include lattice dynamics of intercalated graphite, structure and dynamics of spin glasses, random field systems, polarized-beam studies of paramagnetism, metallic superlattices, proton diffusion in biological systems, and collagen periodicity in bones.

LABORATORIES

OAK RIDGE NATIONAL LABORATORY (continued)

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

$415,000 02-2

Investigations of flux-line-lattice arrays, flux flow, flux creep, flux-line defect interactions, and anisotropy in refractory metal alloys and compounds with A15 and B1 crystal structures; small-angle neutron scattering by fluxline lattices in equilibrium and metastable 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 laser quenching of superconductors.

231. SEMICONDUCTOR PHYSICS AND PHOTOPHYSICAL PROCESSES OF SOLAR ENERGY CONVERSION

R. F. Wood, R. B. James, E. Fogarassy, G. E. Jellison,
D. H. Lowndes, F. A. Modine, R. Ruckteschler, R. D. Westbrook,
R. T. Young
Phone: (615)-574-5781

$845,000 02-2

Time-resolved optical and electrical measurements of laser-induced melting and recrystallization; picosecond laser spectroscopy, laser-induced photochemical deposition; thermal and laser annealing of lattice damage in Si and GaAs; laser-induced recrystallization of amorphous layers; fabrication of high-efficiency Si solar cells by laser techniques; effects of point defects, defect clusters, dislocations, stacking faults, and chemical 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 property measurements; dopant concentration profiles, deep-level transient spectroscopy, and absolute quantum efficiency measurements; fabrication of test solar cells; solar cell modeling; thin-film deposition on prepared substrates; chemical vapor deposition of Si on low-cost substrates.

LABORATORIES

OAK RIDGE NATIONAL LABORATORY (continued)

232. FUNDAMENTAL ASPECTS OF METAL FRACTURE

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

$485,000 02-2

Experimental and theoretical investigations to relate phenomena of continuum fracture mechanics to microscopic physical phenomena occurring at a crack tip; in situ transmission electron microscope observations of crack propagation in aluminum, copper, nickel, molybdenum, niobium, tungsten, stainless steel, magnesium oxide, and niobium oxide; crack propagation in metals containing helium bubbles; distribution of dislocations in the plastic zone ahead of crack tip in metals and ceramics; cyclic deformation; ductile-brittle transition in bcc metals; dislocation theory of J-integral; theory of plastic zone with a dislocation-free zone; in situ TEM studies of crack propagation in gaseous (hydrogen) environment.

233. PHYSICAL PROPERTIES OF CERAMICS

F. A. Modine, C. Y. Allison, Y. Chen, G. R. Gruzalski, J. R. Martinelli, E. Sonder, R. A. Weeks
Phone: (615)-574-6287

$685,000 02-2

Transition-metal carbides and nitrides and the 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; techniques include optical and paramagnetic resonance spectroscopies, electrical properties measurements, and laser heating.

234. CHARGE TRANSPORT IN SOLID ELECTROLYTES

J. B. Bates, W. E. Brundage, Y. T. Chu, N. J. Dudney, J. C. Wang
Phone: (615)-574-6280

$405,000 02-2

Kinetics and thermodynamics of the hydration reaction of beta- and beta"-aluminas; effect of intercalated water on electrical properties; composite electrolytes and the mechanisms of ionic transport in multiphase materials; charge and mass transport at metal-dielectric and dielectric-dielectric interfaces; techniques include impedance spectroscopy, transient signal analysis, Raman scattering, infrared absorption, ATR and internal reflection spectroscopy, and electron microscopy; experimental results are interpreted and correlated by means of model calculations.

LABORATORIES

OAK RIDGE NATIONAL LABORATORY (continued)

235. PREPARATION AND CHARACTERIZATION OF RESEARCH MATERIALS

L. A. Boatner, M. M. Abraham, W. E. Brundage, Y. K. Chang
Phone: (615)-574-5492

$650,000 02-2

Development of new techniques for growth of single-crystal research specimens and for advanced materials preparation; techniques for the growth of single crystals with specified geometries; flux growth of single crystals of fast-ion conductors (beta-alumina, beta"-alumina); Czochralski and float-zone growth of crystals of Fe-Ni-Cr alloys (i.e., stainless steels); growth of refractory metal crystals (Ti, V, Zr, Nb, Ta, W, Ir, Re) using electron-beam float-zone technique; rf induction float-zone growth of transition-metal carbides; growth of perovskite-structure oxides ($KTaO_3$, $KTa_{1-x}Nb_xO_3$, CaTiO3) and semiconducting oxides for photoelectrochemical cell electrodes; float-zone and tri-arc growth of crystals of A15 compounds such as V_3Si, V_3Ge, and Ti_3Pt; arc-fusion and flux growth of crystals of high-temperature materials (WC, Y_2O_3, MgO, CaO, SrO); characterization of high-quality single crystals of metals, alloys, and insulators.

236. SMALL-ANGLE X-RAY SCATTERING (see also page D-11)

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

$155,000 02-2

Small-angle X-ray scattering of metals, metallic glasses, precipitates, alloys, polymers, and surfactants; void distributions in oil shale and irradiated metals; dynamic deformation studies of polymers; time-slicing studies of phase transformations. Facilities are available to users through National Center for Small-Angle Scattering Research (NCSASR).

LABORATORIES

OAK RIDGE NATIONAL LABORATORY (continued)

237. THEORY OF CONDENSED MATTER

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

$1,160,000 02-3

Theory of laser annealing, laser-induced diffusion, and nonequilibrium solidification in semiconductors; superionic conductivity and solid electrolytes; lattice dynamics and potential energy calculations of ionic crystals; computer simulation of radiation damage and sputtering; radiation damage analysis procedures; radiation emitted by channeled electrons; reflection of light atoms from surfaces; surface studies with backscattered ions; development of LEED theory and interpretation of LEED data; surface vibrations and relaxation; correlation contributions to surface energy; optical potential for electron spectroscopies; theory of angular effects in photoemission and Auger emission of electrons from surface regions; electron screening; electronic structure of metal surfaces; lattice dynamics of transition metals; magnetism in transition metals; Brillouin zone integration; Heisenberg spin systems; metal-hydrogen interactions; high-temperature oxides and carbides; lattice vibrations in alloys; coherent potential approximation; neutron scattering from crystals, molecular-like impurities in crystals, and alloys; electronic properties of rare-earth and actinide compounds; band structure calculations for metals and insulators; electronic properties of mixed-valent systems; critical phenomena and phase transitions; dynamical properties of fractal systems.

238. X-RAY DIFFRACTION AND ELECTRON MICROSCOPY

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

$850,000 02-4

Structure of intrinsic and induced defects in solids; transmission electron microscopy; synchrotron X-ray scattering; X-ray diffuse scattering; X-ray topography; defect clusters resulting from fast neutron and ion irradiations of metals; pulsed-laser annealing; defects associated with laser and thermal processing of pure and ion-implanted semiconductors; cell structure in doped semiconductors; grain boundaries in semiconductors; high-resolution atomic imaging of defects; structure of displacement cascades in silicon; solid-phase recrystallization in semiconductors; structure of high-temperature metal carbides; defects in high-temperature oxides; anisotropic elastic theory of dislocation loops; computer simulation of electron microscopy images; novel 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 interactions of electrons and X-rays with defects in solids.

LABORATORIES

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

$400,000 02-4

Application of enriched isotopes to the development of new advanced materials; tailoring of materials properties by means of stable and radioactive isotopes; production of isotopically enriched materials for detailed spectroscopic and materials characterization; use of isotopic solids in investigations of polycrystalline ceramics, glasses, single-crystal metals, and dielectrics; studies of physical, chemical, and mechanical properties of isotopic solids by means of optical absorption, electron paramagnetic resonance, Raman scattering, Mossbauer spectroscopy, ion implantation, Rutherford backscattering, and thermal analysis; exploitation of isotopic properties in resolving basic scientific problems; use of isotopes in the development of materials for applications in advanced materials-related technologies.

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

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

$190,000 02-4

Design, construct, test, and operate for users a National Low-Temperature Neutron Irradiation Facility (NLTNIF) at the ORNL Bulk Shielding Reactor (BSR); determine neutronics characteristics in the irradiation cryostat for use at an in-core position and with several radiation modifying devices; provide data acquisition and computer equipment for users; design and construct specialized cryogenic test equipment; provide equipment and procedures for the transfer of irradiated specimens at 4.2 K.

LABORATORIES

OAK RIDGE NATIONAL LABORATORY (continued)

241. SURFACE PHYSICS AND CATALYSIS

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

$960,000 02-5

Studies of crystallographic and electronic structure of clean and adsorbate-covered metal binary alloy and semiconductor surfaces with emphasis on surfaces which either reconstruct or have interplanar spacings different from those of the bulk; combined techniques of low-energy electron diffraction (LEED), positive ion crystallography of surfaces (PICS), photoelectron spectroscopy (PES) using synchrotron radiation, and computer simulations for surface crystallography studies; 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 and intermetallic compounds; 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 (SMAC) FACILITY AND COLLABORATIVE RESEARCH CENTER (see also page D-21)

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

$500,000 02-5

SMAC facility for alteration of materials properties in UHV by ion implantation doping, pulsed-laser processing, and ion beam mixing at sample temperatures from 4-1300 K; in situ materials characterization by ion-beam analysis, ion channeling, electrical measurements, and surface analysis techniques; SMAC facility supports research in the Ion Beam Analysis and Ion Implantation Program and other ORNL divisions; SMAC facility is available to scientists outside ORNL for collaborative research projects through the SMAC Collaborative Research Center.

LABORATORIES

OAK RIDGE NATIONAL LABORATORY (continued)

243. ION BEAM ANALYSIS AND ION IMPLANTATION

B. R. Appleton, C. W. White, M. J. Aziz, J. H. Barrett,
G. M. Beardsley, R. J. Culbertson, G. C. Farlow, E. Fogarassy,
O. W. Holland, E. Kelly, O. E. Schow, J. M. Williams, S. P. Withrow
Phone: (615)-574-6283

$970,000 02-5

Fundamental studies of ion implantation damage and annealing; dynamic annealing during implantation; formation of buried amorphous or insulating layers by implantation; fundamental studies of ion beam mixing; positive ion crystallography of surfaces (PICS); ion-solid interactions (particulary ion channeling); pulsed-laser annealing and rapid solidification; high-speed nonequilibrium crystal growth; investigations of segregation, constitutional supercooling, solute trapping, and precipitate formation; mechanisms limiting maximum substitutional concentrations during rapid solidification; supersaturated substitutional alloys; new metastable phases and amorphous alloys fabricated by ion beam and pulsed-laser processing; rapid thermal annealing; solid-phase epitaxial regrowth; applications of ion implantation doping and pulsed-laser processing to studies of corrosion/catalysis mechanisms, to reduction of friction and wear of metal surfaces, to improvements in hardness and fracture toughness of ceramics, to improvements in high-temperature materials, and to superconducting materials fabrication; ion beam and pulsed-laser mixing in metals, semiconductors, and insulating substrates; ion implantation of surgical alloys; surface smoothing of laser mirrors.

244. RESEARCH AND DEVELOPMENT - ISOTOPE RESEARCH MATERIALS PREPARATION

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

$340,000 02-5

Research and development of preparative techniques applicable to isotopic materials. Stable and radioactive isotopes 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 conventional spray calcination, nonconsumable arc melting, vacuum distillation, conversion of organic precursors to oxide films and solid forms, He implantation in metals, and general inorganic chemical processing. In-house characterization methods include X-ray diffraction and fluorescence, metallographic and ceramographic sample preparation, optical microscopy, scanning electron microscopy with energy dispersion X-ray spectrometry, differential thermal analysis, microgravimetric determinations, thermal conductivity determinations, in-situ film thickness monitoring, and sophisticated radiation counting methods.

LABORATORIES

OAK RIDGE NATIONAL LABORATORY (continued)

Chemistry Division - 03 -

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

245. CHEMICAL STRUCTURE OF ENERGY RELATED MATERIALS

W. R. Busing, B. K. Annis, G. M. Brown, E. Johnson, A. H. Narten, D. W. Noid, W. E. Thiessen
Phone: (FTS) 624-4976 or (615)-574-4976
$850,000 03-1

Atomic and molecular arrangements in crystals and in liquids determined by neutron and X-ray diffraction studies; atom-atom pair correlation functions for liquids; precise electron densities in crystals; neutron spectroscopy; development of synchrotron radiation facilities. Computational methods for dynamic correction of neutron scattering intensities; improvement of statistical mechanics techniques for application to ionic solutions or molten salts; use of computational models to interpret the effects of intermolecular packing forces on the geometry of molecules in crystals; calculation of physical properties of crystals. Materials studied include amorphous metal alloys, compounds which are potential catalysts for hydrogenation and hydrogen production, molten salts, aqueous lanthanide and actinide solutions, and silicate minerals of the earth's mantle.

246. HIGH TEMPERATURE CHEMISTRY AND THERMODYNAMICS OF STRUCTURAL MATERIALS

C. E. Bamberger, J. Brynestad, G. M. Begun, L. Maya
Phone: (FTS) 624-4944 or (615)-574-4944
$678,000 03-2

Synthesis of high-purity structural ceramic compounds by novel reactions; heterogeneous (gas-solid) reactions that yield extremely fine powders; reactions of titanium and titanium chlorides with gaseous BCl_3 to yield TiB_2 powder with particles size of 100 nm or less; chemistry of precursors formed at low temperatures; electrochemistry of aluminum in liquid ammonia; reactions of gaseous HF with commercial SiC to remove oxide contamination; reaction thermodynamics and mechanisms; compaction and sintering studies.

LABORATORIES

OAK RIDGE NATIONAL LABORATORY

Chemical Technology Division - 03 -

R. G. Wymer - Phone (FTS) 624-6275 or 615-574-6275

247. LOCALIZED CORROSION AND STRESS CRACKING PHENOMENA RELATED TO ENERGY TECHNOLOGIES

F. A. Posey, A. L. Bacarella, H. R. Bronstein, Gilbert M. Brown, E. J. Kelly, C. E. Vallet
Phone: (FTS) 624-5022 or (615)-574-5022
$730,000 03-3

Mechanism of the hydorgen evolution reaction on titanium; theoretical and experimental studies on initiation and propagation of crevice corroison of titanium; autopassivation of titanium in localized corrosion; hydrolysis, speciation, and other medium effects on interfacial reaction kinetics in concentrated aqueous electrolytes encountered in localized corrosion; application of photoacoustic spectroscopy coupled with electrochemical measurements to in situ corrosion studies (film formation and breakdown, surface concentration and identity of reaction intermediates, etc.); theory of response of occluded corrosion systems to impedance and transient measurements.

248. THERMODYNAMICS AND SENSITIVITY ANALYSES INVOLVING ENERGY-RELATED MATERIALS

T. B. Lindemer, T. M. Besmann, C. A. Culpepper
Phone: (FTS) 624-6275 or (615)-574-6850
$360,000 03-2

This program is designed to measure and interpret the chemical thermodynamic properties of the extensive solid solutions present in the U-Pu-RE-O systems, where RE represents the lanthanides. The thermodynamic properties of the actinide oxides are being studied experimentally and theoretically, as are general mathematical theories for determining chemical equilibrium in multicomponent systems. Much of this work is generally applicable to the prediction of the properties of nonstoichiometric oxide solid solutions and of multicomponent chemical systems.

LABORATORIES

OAK RIDGE NATIONAL LABORATORY (continued)

249. CHEMICAL ENGINEERING RESEARCH

C. H. Byers, D. F. Williams
Phone: (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 and those found in coal conversion streams. Viscosities, diffusivities, and vapor-liquid equilibrium at high pressures and temperatures. Crystallization and growth of monodispersed seed materials, particle size analysis.

LABORATORIES

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

Materials Science Division - 01 -

S. D. Dahlgren - Phone (FTS) 444-0120 or 509-376-0120

260. HIGH TEMPERATURE CORROSION AND ELECTROCHEMICAL INTERACTIONS IN CERAMICS

J. L. Bates, D. D. Marchant
Phone: (509)-375-2579 or (509)-375-2997

$265,000 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-silicates 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 and diffusion near reaction interfaces from elemental distributions and grain boundary character using high-resolution, quantitative EDX, electron microprobes and STEM, coupled with optical microscopy, TEM, SEM and AES and related surface analyses.

261. SPUTTER DEPOSITED AMORPHOUS SEMICONDUCTORS

P. M. Martin, W. T. Pawlewicz
Phone: (509)-375-2076

$100,000 01-1

Study of the effects of composition and microstructure on the electrical, optical and mechanical properties in sputtered thin film amorphous semiconductors. Development of models of reaction kinetics and film-plasma interactions occurring during the reactive sputtering process. Exploration of relationships between local bonding and configurations, stoichiometry and microstructure. The properties of SiN:H and Si-N-O being investigated. Measurements of intrinsic stress, bonding, phase composition and stoichiometry. Electrical property determinations of temperature dependent resistivity, Hall effect, C-V and I-V characteristics. Optical properties under investigation are refractive index, infrared vibrational absorptions and the fundamental interband absorption edge. Measurement techniques: optical and infrared spectroscopy, Raman spectroscopy, electrical transport measurements, C-V and I-V analysis, XPS, X-ray diffraction and X-ray fluorescence.

LABORATORIES

PACIFIC NORTHWEST LABORATORY (continued)

262. FUNDAMENTAL STUDIES OF STRESS CORROSION AND CORROSION FATIGUE MECHANISMS

R. H. Jones, M. T. Thomas, D. R. Baer, M. J. Danielson
Phone: (509)-376-4276

$360,000 01-2

Investigation 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 of Fe, Ni and FeCrNi are 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. Effect of plastic strain and various gaseous environments (O_2, H_2O and H_2O + Cl) on the quantity and distribution of surface adsorbates on Fe, Ni and FeCrNi is being studied by Auger Electron Spectroscopy using an in-situ straining stage.

263. OXIDATION AND CORROSION RESISTANT FINE-GRAINED MATERIALS

J. T. Prater, D. R. Baer
Phone: (509)-375-6905

$65,000 01-3

Investigations of the mechanisms controlling the high-temperature corrosion of sputter-deposited fine-grained materials. Oxidation and sulfidation studies on stainless steel in CO-CO_2 and CO-CO_2-H_2S gaseous environments at 800 to 1000C. AEM, micro-focus x-ray diffraction and mechanical tests are being used to determine the effect alloy grain size, alloying additions, and gaseous environment have on scale microstructure, scale adherence and scale cracking behavior. AES, XPS, and nuclear microprobe measurements are employed to determine the diffusion and chemical state of elements at the alloy surface during the corrosion process.

LABORATORIES

PACIFIC NORTHWEST LABORTORY (continued)

264. LEACHING OF GLASS AND CERAMICS

G. L. McVay, L. R. Pederson, D. S. Goldman
Phone: (509)-375-3762

$250,000 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.

265. 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., H. E. Kissinger, R. Wang, W. J. Weber
Phone: (FTS) 444-3124

$650,000 01-4

Evaluation of radiation damage mechanisms in metals and non-metals; irradiation of metals using heavy-ion and neutron bombardment; analyses using analytical electron microscopy, positron annihilation, rate theory microstructural modeling; in-situ irradiation creep testing; effects of irradiation and substructure on creep, recovery, recrystallization, defect microstructures and hardening; pulsed irradiation effects on microstructures; effects of primary damage on amorphous and crystalline phase stability and corrosion resistance; studies of ferritics, nickel, molybdenum, amorphous metals, and ordered intermetallic compounds. Dose and dose rate dependence of damage ingrowth in non-metallic solids resulting from internal alpha decay events, external ion bombardment, and gamma irradiation. Characterization of localized defect states in glasses and crystals by vibrational Raman spectroscopy and optical absorption techniques. Kinetic studies of damage ingrowth and annealing phenomena using x-ray diffraction, electron microscopy, and bulk swelling determinations. Model development for the damage state in insulators with an emphasis on radiation induced structural changes in glassy silicates and phosphates.

LABORATORIES

PACIFIC NORTHWEST LABORATORY (continued)

266. SPUTTERING PARAMETER INFLUENCES ON MATERIAL STRUCTURE AND BEHAVIOR

R. W. Knoll
Phone: (509)-375-6902

$90,000 01-5

Synthesis of metallic alloys, ceramic, and dielectric materials by sputter deposition and reactive sputtering. Characterization of microstructure, structure and phase stability, using x-ray diffraction, TEM, SEM, AES, thermal analysis, as well as electrical and optical measurements. Emphasis on unique nonequilibrium or metastable phases and composites. Definition of the deposition process and relations between process parameters and material characteristics. Material systems include rare earth/transition metal alloys, refractory metal alloys, binary and ternary oxides.

267. THIN FILM OPTICAL MATERIALS

W. T. Pawlewicz, J. W. Griffin, P. M. Martin
Phone: (509)-375-2074

$270,000 02-2

Measurement, modeling and improved understanding of the optical and materials properties of oxides, nitrides and elemental semiconductors in single and multilayer thin-film form. Materials synthesis by reactive sputtering. Optical properties studied: absorption, scattering, optical homogeneity and isotropy, spectral dependence of complex refractive index, and fundamental interband and lattice vibrational absorption edges. Related materials properties: structure, microstructure, bonding in amorphous materials, stoichiometry, composition, purity, surface topography and mechanical stress. Optical measurement techniques: total integrated scattering, angular scattering distribution, reflectance and transmission spectrophotometry, photoacoustic spectroscopy, laser interferometry and ellipsometry. Materials characterization emphasis on X-ray diffraction, Raman spectroscopy and scanning transmission microscopy. Performance environments: high-power lasers, solar radiation, temperature cycling and humidity exposure.

LABORATORIES

SANDIA NATIONAL LABORATORIES
P. O. Box 5800
Albuquerque, New Mexico 87185

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

275. ION IMPLANTATION AND DEFECTS IN MATERIALS

P. S. Peercy, 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, F. G. Yost, R. B. Diegle, N. R. Sorensen
Phone: (FTS) 844-4309 or (505)-844-4309

$850,000 01-3

Ion implantation in conjunction with laser and electron-beam annealing to form metastable and equilibrium states within the near-surface regions of metals, semiconductors, and insulators. Microscopic characterization of modified layers by ion-beam depth-profiling, ion channeling, TEM, EPR, AES, ESCA, optical absorption and X-ray scattering. Studies of kinetics of transient laser/electron-beam annealing by time-resolved reflectance and conductance and by calorimetry. Diffusion rates, phase diagrams, and solute-trapping mechanisms in equilibrium intermetallic systems. New metastable crystalline and amorphous alloys produced both by ion implantation and by transient annealing; stability bounds, microstructures, and mechanical and corrosion properties are measured. Ion implantation used to separate structural and chemical effects on corrosion. Methods based on ion implantation and ion beam analysis used to characterize the behavior of hydrogen in metals, including diffusivity, solubility, surface-barrier effects, and trapping by defects, solutes, precipitates and gas bubbles. Fundamental properties of defects and impurities in semiconductors using EPR and optical absorption following controlled introduction by ion implantation. Laser and electron-beam annealing of silicon for the removal of implantation-doping damage, the production of single-crystal silicon on insulators, and to elucidate fundamental aspects of rapid solidification. Refractory amorphous alloys for diffusion barriers or metallization of semiconductors for elevated temperature applications.

LABORATORIES

SANDIA NATIONAL LABORATORIES - ALBUQUERQUE(continued)

276. STRESS CORROSION IN CERAMICS AND SOL GEL TRANSITION IN SIMPLE SILICATES

T. A. Michalske, M. L. Knotek, G. A. Fisk, B. C. Bunker,
K. D. Keefer, D. W. Schaefer, C. J. Brinker
Phone: (FTS) 844-4069 or (505)-844-4069

$500,000 01-2

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

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: (FTS) 844-6653 or (505)-844-6653

$350,000 01-5

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.

LABORATORIES

SANDIA NATIONAL LABORATORIES - ALBUQUERQUE (continued)

278. SURFACE PHYSICS RESEARCH AND STIMULATED DESORPTION

M. L. Knotek, J. E. Houston, D. Jennison, G. Kellogg, R. R. Rye, R. Stulen, J. Kelber, A. Burns
Phone: (FTS) 844-2272 or (505)-844-2272

$690,000 02-2

Broad program with wide technological and scientific impact involving experimental and theoretical studies aimed at understanding the interaction of solid surfaces with their environment; unique local surface Properties obtained by exploiting Auger Electron Spectroscopy, Photon and Electron Stimulated Desorption Spectroscopies, the Pulsed Laser Atom-Probe technique and Low Energy Electron Loss Spectroscopy. Studies from those on the chemical nature and local electronic properties of intermediate species adsorbed on catalytic surfaces to work determining the molecular properties controlling initiation sensitivity in aromatic explosives; from studies of the chemistry of oxide surfaces and its relationship to catalytic support interactions and stress corrosion cracking in glasses and ceramics to work dealing with the effect of microscopic surface defects on the interaction of adsorbates with metal surfaces. Theoretical work complements several of these experimental efforts by elucidating the physics of the processes involved to provide a better understanding of the relationship between the results and fundamental material properties.

279. ORGANIC CONDUCTORS AND SUPERCONDUCTORS

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

LABORATORIES

SANDIA NATIONAL LABORATORIES - ALBUQUERQUE (continued)

280. CHEMICAL VAPOR DEPOSITION AND SURFACE PHOTOKINETIC RESEARCH

A. W. Johnson, W. G. Breiland, P. Ho, M. E. Coltrin,
J. R. Creighton, P. J. Hargis, M. E. Riley
Phone: (FTS) 844-8782 or (502)-844-8782

$410,000 03-3

Studies of important vapor-phase reactions and nucleation processes during CVD deposition under conditions used to fabricate photovoltaic cells, corrosion-resistant coatings, and semiconductor devices. Measurements of major and minor species densities, gas temperatures, fluid flows, and gas-phase particulate distributions using laser Raman and Mie scattering and laser induced fluorescence. Test of our predictive model, which includes chemical kinetics and fluid dynamics. Study and development of laser CVD, laser photochemical deposition, laser-based physical deposition, 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 during deposition and etching. Development of model for combined laser, admolecule, and surface dynamics.

LABORATORIES

SANDIA NATIONAL LABORATORIES
Livermore, California 94550

D. Hartley - Phone (FTS) 532-2747 or 412-422-2747

290. PROTECTIVE BARRIERS AND COATINGS FOR COMBUSTION-RELATED MATERIALS

R. E. Palmer, J. C. Hamilton, A. S. Nagelberg
Phone: (FTS) 532-3126 or (415)-422-3126
$390,000 01-1

Investigations in real time of gas-solid reactions, emphasizing hot corrosion and microstructural effects in attack of metals and ceramics. Studies of molten alkali sulfate-vanadate attack of yttria-stabilized zirconia. Role of surface microstructure on reaction processes determined in situ with a hot stage on a Raman microprobe. Temporally resolved corrosion studies with mixed gas-phase oxidants in environmental cells. Program relies heavily on Raman spectroscopy to characterize reaction conditions difficult to analyze by post-exposure techniques.

291. GASES IN METALS

M. I. Baskes, G. J. Thomas, M. S. Daw
Phone: (FTS) 532-3226 or (415)-422-3226
$249,000 01-2

Investigations of the behavior of hydrogen and helium in metals involving joint theoretical and experimental research. Experimental techniques include electron microscopy, positron annihilation, mechanical property measurements, and small angle neutron scattering, applied to tritiated metals and also metals implanted with helium below the damage threshold. Theoretical effort on spontaneous lattice damage by helium and on helium-dislocation interactions. 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 and the effects of hydrogen and trapping of hydrogen by impurities and alloying additions.

LABORATORIES

SANDIA NATIONAL LABORATORIES - LIVERMORE (continued)

292. MECHANISMS OF HYDROGEN EMBRITTLEMENT - EFFECTS OF GASEOUS VERSUS ELECTROCHEMICAL CHARGING

S. L. Robinson, N. R. Moody, J. C. Farmer
Phone: (FTS) 532-2209 or (415)-532-2209

$120,000 01-2

Investigation of electrochemical charging with hydrogen to simulate gaseous hydrogen environments by comparing electrochemically and gas phase charged FCC alloys. Electrochemical charging experiments using poisoned, unpoisoned and tritium labelled electrolytes and gas phase charging experiments using hydrogen and tritium atmospheres. Electrochemical techniques of cathodic polarization, cyclic voltammetry and impedance to characterize surface response to charging conditions and solutions. Ion beam profiling determines hydrogen depth profiles, effective hydrogen diffusivities, and effective hydrogen fugacities. Autoradiography of tritium charged samples characterizes hydrogen interactions with microstructural features. Scanning and transmission electron microscopy techniques determine the type of microstructural damage induced by electrochemical and gas phase charging techniques and the conditions which induce damage.

293. THIN SURFACE LAYER REACTIONS

R. E. Palmer, R. J. Anderson, J. C. Hamilton
Phone: (FTS) 532-3126 or (415)-422-3126

$230,000 02-2

In situ studies of the early stages of oxide and other compound formation on metal surfaces. Characterization of bond structure of few-monolayer surface films, time evolution of this bond structure to crystalline structure, and atomic mobility during film thickening. Studies of the role of temperature and oxygen partial pressure in rearrangement rates and final film structures. Primary measurement technique is spontaneous Raman spectroscopy, complemented by Auger spectroscopy and LEED. Development of greater capability of Raman for detecting very thin, possibly monolayer, or weakly scattering oxide films by means including electronic resonant enhancement and state-of-the-art instrumentation. Raman spectroscopy of films tagged with oxygen isotopes to determine reaction mechanisms.

LABORATORIES

SOLAR ENERGY RESEARCH INSTITUTE
1617 Cole Boulevard
Golden, Colorado 80401

C. S. Smith - Phone (FTS) 327-7180 or 303-231-7180

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, P. Schissel, J. D. Webb, J. R. Pitts
Phone: (303)-231-1240

$290,000 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 polymethylmethacrylate, polycarbonate, and polypropylene in contact with copper and silver oxides, chlorides, and sulfides 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, λ, GPC, XPS, ISS, SIMS, AES, SEM, 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

$130,000 02-3

Theoretical study of electronic and structural properties of new semiconductors for optoelectronic applications to clarify electronic properties, predict new materials, characterize structurally-driven optical and electronic phenomena. Systems: ternary chalcopyrites ABC_2 (A=Cu, B=Al, Ga, In, C=S,Tr); ternary pnictides ABC_2 (A=Zn, B=Si, Ge, Sm, C=P, As); and ternary alloys of binary semiconductors $A_xB_{1-x}C$. Theoretical techniques: all-electron Mixed Basis Potential Variation (MBPV) band structure method, and non-local pseudopotential method. Study of the properties of deep defects in semiconductors to establish chemical trends in 3d impurity levels, predict hitherto unobserved levels, clarify role of deep impurities on material characteristics as affecting their use in optoelectronic devices. Systems: Si, III-V and II-VI semiconductors. Theoretical techniques: Quasi Band Crystal Field (QBCF) Green's function method, and Modified ("effective Δ") multiplet theory.

LABORATORIES

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

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

298. RESEARCH AND DEVELOPMENT OF SYNCHROTRON RADIATION FACILITIES
(see also page D-13)

A. I. Bienenstock, G. S. Brown, and H. Winick
Phone: (FTS) 461-9300 or (415) 854-3300
$700,000 02-2

Research and development on insertion devices and other equipment and facilities to improve research capabilities of synchrotron radiation sources.

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. TRANSPORT IN SOLID ELECTROLYTES CONTAINING A DISPERSED SECOND PHASE

J. B. Wagner
Center for Solid State Science
Phone: (602)-965-6959, 4544

$84,917 (18 Months) 01-3

Characterization of contribution of number and mobility of ionic charge carriers and of space charge layers to conductivity increase mechanisms in a AgI or CuCl matrix containing a second phase such as silica, MgO, flyash, etc. Role of aliovalent doping of the matrix phase. Behavioral effects due to moisture and to added dielectrics such as alcohols or hydrocarbons. SEM, variable frequency ac conductivity, and dc polarization analysis.

302. IMAGING OF SURFACES AND DEFECTS OF CRYSTALS

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

$105,879 02-2

Techniques of microdiffraction, imaging of surfaces using reflected diffracted electrons and electron energy loss spectroscopy applied to study of near-amorphous thin films of oxides and other corrosion products on metal surfaces and investigations of surface reactions of various ceramic oxides. Allied development and exploration of new and improved electron-optical techniques for study of surface structures and reactions and the influence of crystal defects.

UNIVERSITY OF ARIZONA
Tucson, Arizona 85721

303. ARTIFICIALLY LAYERED SUPERCONDUCTORS

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

$75,141 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; 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
505 King Avenue
Columbus, OH 43201

304. MULTIAXIAL STRESS RESPONSE OF CERAMICS

A. R. Rosenfield
Phone: (614)-424-4353
D. K. Shetty
Phone: (614)-424-4353
S. G. Sampath
Phone: (614)-424-4353
W. H. Duckworth

$160,000 01-5

Response of ceramic materials to multiaxial stress states. Consideration of: (a) surface conditions, (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 isotopic and materials directionality is eliminated. Relationship of stress-state effects to stress-intensity factor, effects of tensile and shear stresses parallel to an artificial crack and effect of stress ratios on strength in ceramic specimens containing natural flaws to evaluate statistical (Weibull) descriptions of strength. Material characterization, fractrography, 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, SiC, Si_3N_4, and glass-ceramics, and partially stabilized ZrO_2.

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

305. X-RAY SPECTROSCOPIC INVESTIGATION OF METAMICTIZATION & ANNEALING IN CRYSTALLINE PHOSPHATES, SILICATES AND COMPLEX TI-NB-TA OXIDES

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

$80,030 01-1

Detailed examination of the near neighbor site geometries of metal atoms in metamic minerals (e.g., A (U,TH) and B (Ti,Nb,Ta) site cations) as determined by extended X-ray absorption fine structure (EXAFS) 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) which would be subject to the same processes of radiation damage and geochemical alteration in applications as a primary host for radioactive wastes.

BRANDEIS UNIVERSITY
415 South Street
Waltham, MA 02254

306. TWO-DIMENSIONAL COLLOIDAL SYSTEMS

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

$43,955 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.

BROWN UNIVERSITY
Providence, RI 02912

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

R. J. Asaro
Div. of Engineering
Phone: (401)-863-1456
J. Gurland
Div. of Engineering
Phone: (401)-863-2628
A. Needleman
Div. of Engineering
Phone: (401)-863-2863
C. F. Shih

$237,000 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.

BROWN UNIVERSITY (continued)

308. 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

$93,500 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 conditions; dislocation interaction with point effects; metals studied - Al, Fe, Nb, Ti, Zn.

309. 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

$94,950 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.

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

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

$80,444 02-2

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

CALIFORNIA INSTITUTE OF TECHNOLOGY
Pasadena, CA 91125

311. STUDIES OF ALLOY STRUCTURE AND PROPERTIES

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

$270,000 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 investigating 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.

312. MELTING IN ADSORBED FILMS

D. Goodstein
Div. of Physics, Mathematics, and Astronomy
Phone: (213)-356-4315

$93,000 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

313. RADIATION DAMAGE AND STABILITY OF NUCLEAR WASTE STORAGE MATERIALS

D. G. Howitt
Dept. of Mechanical Engineering
Phone: (916)-752-1164, 0580

$97,000 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.

UNIVERSITY OF CALIFORNIA/DAVIS (continued)

314. DEFORMATION MECHANISMS AND FAILURE MODES IN SUPERPLASTICITY

A. K. Mukherjee
Dept. of Mechanical Engineering
Phone: (916)-752-1776

$59,746 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.

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

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

$66,000 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. Study of state of division of oxide ceramic resulting from the decompostion 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.

UNIVERSITY OF CALIFORNIA/IRVINE
Irvine, CA 92717

316. RAMAN SPECTROSCOPY OF MOLECULAR ADSORBATES

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

$140,000 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.

317. SURFACE EXCITATIONS AND THEIR INTERACTION WITH LOW ENERGY ELECTRONS

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

$103,000 02-2

Theory of electron energy loss spectroscopy (EELS) and other inelastic scattering at surfaces. Vibrational properties of isolated adatoms and ordered overlayers on metal surfaces, with emphasis on quantitative comparisons with experiment. Role of image potential in large-angle EELS and in LEED studies. Large-angle inelastic scattering from substrate phonons. EELS spectral densities at large wave vector. Surface relaxation, anharmonicity, and surface lattice dynamics. This program strongly coupled to that of S. Y. Tong, University of Wisconsin-Milwaukee.

UNIVERSITY OF CALIFORNIA/SAN DIEGO
La Jolla, CA 92037

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

M. B. Maple
Dept. of Physics
Phone: (714)-452-3969

$292,000 02-2

An experimental program to investigate the coexistence of superconductivity and magnetism. A-15's, ternary molybdenum chalcogenides, and other high T_c superconductors of primary interest. Properties of rare earth compounds such as $ErRh_4B_4$ and $ErMo_6Se_8$ studied in order to understand re-entrant and coexistence phenomena. Collaborative efforts study valance instabilities in Ce compounds and the superconductivity of graphite intercalated with potassium. Studies of the oscillatory oxidation of CO on Pt using LEED and Auger techniques and of metallic thin film oxidation using electrical resistance.

319. 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

$157,195 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 are established and the physical mechanisms and conditions necessary for the formation of a specific reaction product are determined. Different metal-Si systems are investigated; sample configurations include single metal layer on Si bilayers, multi-layers, and alloy thin film structures. Primary experimental tools are 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 and involves interaction with Oak Ridge National Laboratory.

UNIVERSITY OF CALIFORNIA/SAN DIEGO (continued)

320. RESEARCH ON THE THERMOPHYSICAL PROPERTIES OF MATERIALS

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

$146,214 02-5

Fundamental investigations in thermal physics: (a) quantitative scientific properties of intrinsically irreversible acoustic engines, of other "natural engines" based on the same principles, and of engines using liquid working substance; (b) thermal convection in dilute solutions of ^{3}He in superfluid ^{4}He emphasizing quantitatively the steady convection, highly periodic oscillatory convection, and both the deterministic and stochastic chaos which can develop; (c) the production of spin polarized atomic hydrogen isotopes from a low temperature source together with measurement of physical properties using magnetosound; and (d) study of magnetism in superfluid ^{3}He-A, especially ferromagnetism in zero magnetic field and magnetic anisotropy in small applied fields.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA
Santa Barbara, CA 93106

321. 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

$130,000 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 after development of techniques and facilities.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA (continued)

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

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

$109,629 02-3

Theory of pattern formation in systems far from equilibrium. Specific studies of boundary-layer model of dendritic solidification, theory of pattern selection in directional solidification of alloys, and statistical theory of the kinetics of phase separation. The pattern-forming processes studied of primary importance in the design of metallurgical materials, but applications in other areas also considered.

323. 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

$160,000 (21 Months) 02-3

Development of stochastic numerical techniques for simulating many-body problems where the particles obey Fermi statistics. One-dimensional systems investigated considering various electron-phonon interactions to further the fundamental understanding of conducting polymers. One-dimensional chains of quantum mechanical spins studied with application to spin glasses and pseudo random spin systems such as $CeNiF_3$. Correlation effects and frequency dependent transport considered to test the validity of theoretical approximations such as the Pade and Pade-conformal map techniques. Consideration of many-fermion systems in two and three spatial dimensions.

CARNEGIE INSTITUTION OF WASHINGTON
Washington, DC 20008

324. STUDY OF THE PROPERTIES OF HYDROGEN AT STATIC PRESSURES OF ONE MEGABAR

P. M. Bell
Geophysical Laboratory
Phone: (202)-966-0334
H. K. Mao
Geophysical Laboratory
Phone: (202)-966-0334

$60,000 02-2

Investigations of the hydrogen isotopes, helium, neon, argon, carbon dioxide, methane and other simple gases under very high prssure. Hydrogen studies at static pressure above 2 Mbar. Laser Raman scattering studies of the molecular bonding phenomena and the elastic constants as a function of pressure in deuterium. Further improvement to the Diamond Anvil Cell technique. The Raman and Infrared spectra, Brillouin and X-ray scattering measurements on solid hydrogen and solid argon.

CARNEGIE MELLON UNIVERSITY
Pittsburgh, PA 15213

325. THE EFFECT OF STRESS ON PRECIPITATE MORPHOLOGY

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

$92,211 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.

CARNEGIE MELLON UNIVERSITY (continued)

326. THE ROLE OF PASSIVE SURFACE FILMS ON CORROSION FATIGUE CRACK

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)-578-2711
G. W. Warren
Dept. of Metallurgical Engineering and Materials Science
Phone: (412)-578-3517

$104,599 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

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

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

$142,000 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.

CASE WESTERN RESERVE UNIVERSITY (continued)

328. COUPLED DIFFUSION PHENOMENA

A. R. Cooper
Dept. of Metallurgy and Materials Science
Phone: (416)-368-4224

$66,756 (24 Months) 01-3

Study of rate processes, e.g., precipitation, dissolution, and phase separation in multicomponent systems at high temperatures. Study of transport processes and thermodynamics in multicomponent molten silicate systems, and kinetics of these processes in such systems. Relation of the inter-diffusion coefficient matrix to the individual ionic species mobilities or self-diffusion coefficients. Work focused on systems K_2O-SrO-SiO_2 and CaO-Al_2O_3-SiO_2. Ultimate goal is a sufficiently well-documented understanding of such transport processes that will be useful for prediction of behavior in the many high temperature processes that involve molten silicates.

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

329. 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

$161,314 02-3

Theoretical research on problems relevant to both elementary particle physics, through quantum field theory, and condensed matter physics, via the statistical mechanics of phase transitions. Topics of current interest: non-linear dynamical systems and the transition to chaos, dendritic growth, parallel processing computers as statistical mechanical systems, chiral symmetry breaking in lattice gauge theories, quantized string theory (free and interacting), and problems of chial fermions in lattice theories.

CLARK COLLEGE
Atlanta, GA 30314

330. 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

$93,910 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 electrect 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 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

331. 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

$155,718 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

332. 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

$188,000 (18 Months) 02-2

Quasi-elastic light scattering (QELS), microscopy, and various other optical techniques used to study charged colloidal particle suspensions (CCPS) in thin films, in monolayers, and on bilipid membranes. Examination of melting/crystallization dynamics in CCPS films, supercooling of CCPS liquid films, recovery from electric field induced non-equilibrium states in CCPS films, monolayers and membranes, melting/crystallization, diffusion, order-disorder phenomena for CCPS in monolayers and on membranes, and development of a model of the interaction between colloidal particles in monolayers and on membranes. Also the application of innovative QELS techniques to study the transition to two dimensional behavior of the critical dynamics of thin fluid films.

COLUMBIA UNIVERSITY
New York, NY 10027

333. DEFECT INTERACTIONS AT HIGH CONCENTRATION IN SOLID OXIDE ELECTROLYTES

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

$87,295 01-3

Defects and their interactions in oxygen-ion solid electrolytes, with special emphasis on ceria-based materials doped with divalent and trivalent cations. Techniques used include ionic conductivity, dielectric relaxation, anelastic relaxation, neutron diffraction and scanning transmission electron microscopy. Defect interactions in trivalent-doped (M^{3+}) ceria and effect of M^{3+} ion radius. Role of silicon phases in producing electrical blocking at grain boundaries. Steps that control the electrode reaction, particularly at Pt electrodes. Protonic conduction studies in $SrCeO_3$, and $KTaO_3$.

UNIVERSITY OF CONNECTICUT
Storrs, CT 06268

334. THE FATIGUE BEHAVIOR OF FERRITIC STEELS AT ELEVATED TEMPERATURES

A. J. McEvily
Dept. of Metallurgy and Institute of Materials Science
Phone: (203)-486-2941

$60,540 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.

335. ELECTRODE STUDIES IN MOLTEN SALTS

O. F. Devereux
Dept. of Metallurgy and Institute of Materials Science
Phone: (203)-486-4620

$47,611 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.

336. INVESTIGATION OF ROLE OF SUBSURFACE ZONES IN WEAR OF MATERIALS

R. Solecki
Dept. of Mechanical Engineering
Phone: (203)-486-2366

$89,500 (24 Months) 01-5

Experimental characterization of the formation, composition and morphology of both subsurface zones and wear debris for materials pairs making solid contact both in sliding and repetitive impact modes; experimental investigation of the roles of nominal contact stress, relative sliding velocity and effective contact stiffness of subsurface zone formation, composition and morphology; analytical prediction of the equilibrium configuration of subsurface morphology for a work hardening elastoplastic material subject to given load cycling and temperature distributions; model development which allows prediction of composition and morphology of subsurface zones for selected materials subjected to both sliding and impulsive contact; and postulation and experimental investigation of in situ development of wear resistance.

UNIVERSITY OF CONNECTICUT (continued)

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

$61,172 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 include 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

$92,900 (20 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

$99,000 01-1

Study of the effect of geometry and composition of interfaces on interfacial mobility in ionic and covalent solids. Concerns include (a) misorientation between grains and boundary plane orientation, (b) geometry of interfacial dislocations and steps, (c) interfacial chemistry including local segregation and nonstoichiometry, and (d) 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. DIFFRACTION AND MICROSCOPY STUDIES OF THE STRUCTURE OF GRAIN BOUNDARIES IN FE, FE-BASE ALLOYS, AND CERAMIC MATERIALS

S. L. Sass
Dept. of Materials Science and Engineering
Phone: (607)-256-5239

$174,000 01-1

Investigation of grain boundary structure of BCC metals and ceramics using transmission electron microscopy and x-ray diffraction techniques; study of the influence of segregation on the structure of grain boundaries in Fe-base alloys; study of facet structure of tilt grain boundaries in NiO; model diffraction observations from grain boundary region to determine changes in plane spacing normal to interface in NiO and MgO; relation of structural observations on grain boundaries to mechanical properties.

341. AN INVESTIGATION OF MECHANICAL BEHAVIOUR OF POLYCRYSTALLINE SOLIDS

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

$190,000 01-2

State-variable description of nonelastic deformation and related phenomena in polycrystalline solids. Extensive use is made of load relaxation experiments 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.

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

$105,000 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.

CORNELL UNIVERSITY (continued)

343. HIGH TEMPERATURE MECHANICAL BEHAVIOR OF SILICON NITRIDE

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

$99,000 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

$180,800 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 include nucleating agents, crystallinity, particle size, optical perfection, thermal expansion, and refractive index. Spectroscopic properties, radiative transfer and glass-ceramic structure are 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 Ni_3Al ALLOYED WITH BORON

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

$106,109 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

$59,756 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.

UNIVERSITY OF DELAWARE (continued)

347. NEUTRON STUDIES OF LIQUID AND SOLID HELIUM

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

$55,000 02-3

A theoretical program to calculate properties of liquid and solid helium for direct comparison with neutron scattering measurements in terms of existing and new models and to propose new experiments. Specific examples include $S(Q,\omega)$ in liquid ^{3}He, the momentum distribution in liquid ^{3}He and solid ^{4}He, and to test the impulse approximation.

UNIVERSITY OF DENVER
Denver, CO 80208

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

P. K. Predecki
Dept. of Chemistry
Phone: (303)-871-2141

$79,359 01-3

Lattice thermal expansion measurements will be carried out on cordierite doped with alkali and akali earth dopants using high-temperature Guinier diffractometry. Selected samples will be investigated further using neutron powder diffraction at the Argonne IPNS. Results will be correlated to reveal the mechanism of expansion in this structure.

349. THE DETECTION OF HYDROGEN ASSISTED CRACK GROWTH

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

$72,700 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.

EMORY UNIVERSITY
Atlanta, GA 30322

350. FAR INFRARED STUDIES OF SUPERCONDUCTING A-15 STRUCTURES, NBN AND NB

S. Perkowitz
Physics Dept.
Phone: (404)-329-6584

$43,901 (24 Months) 02-2

Optical techniques in the far infrared region will be used to explore the basic superconducting behavior of the high temperature superconductors V_3Si, Nb_3Ge, Nb and granular NbN. Such spectroscopy will yield accurate gap values, information about the temperature dependence of superconducting properties, values of the electron-phonon spectral function and insight in to grain-to-grain coupling in inhomogeneous geometries. These results will be used to calculate basic superconducting parameters such as the coupling constant and the transition temperature, T_c, with the aim of explicating the underlying physics of superconductivity.

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)-392-1461
C. Batich
Dept. of Materials Science and Engineering
Phone: (904)-392-1461

$115,000 01-3

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

UNIVERSITY OF FLORIDA (continued)

352. FIELD-ION MICROSCOPY AND SPECTROSCOPY OF HYDROGEN IN METALS

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

$76,290 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 in situ implantation at ~40-50 K followed by IAP analyses.

353. 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

$94,000 03-1

The objectives of the proposed research program are to study graft copolymerization of vinyl monomers to polysaccharides, to determine grafting efficiencies, and to determine the structure and properties of the copolymers. In support of these objectives, a variety of model polymers will be synthesized (a) which contain the specific reactive functional groups of the polysaccharide repeating unit, (b) which possess controlled branching sites in order to simulate highly branched polysaccharide grafted copolymers, and (c) which contain macrocyclic units to aid in establishing viscosity-structure relationships.

FRANKLIN INSTITUTE
20th and Parkway
Philadelphia, PA 19103

354. PHYSICS OF HIGHLY ANISOTROPIC MATERIALS

S-T. Chui
Physics Dept.
Phone: (302)-738-8115

$25,005 02-3

Theoretical research on instabilities and elementary excitations associated with correlations in highly anisotropic (mainly quasi-one-dimensional) materials. Principal subject areas: spin and charge density wave relationships, correlations in half filled bands, solitons and Hubbard model excitations, and superconductivity in one-dimensional

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

$159,000 02-3

Theoretical studies of surface phenomena toward fundamental understanding of processes which govern the properties of material surfaces, especially: surface reactivity, surface crystallography, electronic and vibrational structure, dynamical processes, phase transformations and phase changes and the properties of interfaces. Emphasis on surface defects, heterogeneities and reaction mechanisms, surface melting and solidification.

HARVARD UNIVERSITY
Pierce Hall
Cambridge, MA 02138

356. 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

$120,000 02-2

Time-of-flight measurements in the nanosecond to millisecond regime, and other time-dependent studies of amorphous hydrogenated silicon, doped 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.

357. FUNDAMENTAL PROPERTIES OF SPIN-POLARIZED QUANTUM SYSTEMS

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

$260,000 (18 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 to be sought and, if found, characterized.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

372. BASIC MECHANISMS OF THE OXIDATION OF METALS AND ALLOYS

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

$145,000 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.

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

L. W. Hobbs
Ceramics and Materials Science Dept.
Phone: (617)-253-6835

$141,103 01-4

Fundamental research to characterize the irradiation stability and radiation damage microstructure 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, $Ca(Zr,Pu)Ti_2O_7$, titanate pyrochlores, SiO_2, GeO_2, $ZrSiO_4$. Neutron, ion and electron irradiation damage will be studied, including the effects of massive recoil nuclei and fission fragments.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

374. INTERFACIAL AND COLLOIDAL ASPECTS OF AQUEOUS SUSPENSIONS CONTAINING OXIDIC POWDERS

A. Bleier
Dept. of Materials Science and Engineering
Phone: (617)-253-6877

$95,000 (27 1/2 Months) 01-5

Application of colloid-chemical models of single and multimetallic oxides to the processing of their powders. Extension of such models to heterogeneous systems containing more than one particle (composition) type, so as to improve understanding of interfacial complexation and related phenomena which influence dispersibility and packing behavior. Objectives include preparation of model, colloidal single and multimetallic oxides using established synthesis routes, characterization of these oxides using crystallographic, chemical, physical, and surface-chemical procedures, and evaluation of the Davis, James and Leckie model of the electrical double layer.

375. PHYSICS AND CHEMISTRY OF PACKING FINE CERAMIC POWDERS

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

$136,000 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. Generalization controlling the presintered structure of compacts containing 10^{12} particles. Laser diffraction. Photon correlation spectroscopy.

376. LOW TEMPERATURE AND NEUTRON PHYSICS STUDIES

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

$316,930 02-1

Fundamental experiments in neutron diffraction and interferometry using the MIT research reactor, such as the analogue of the famous optical Fizeau experiment in which fringe shifts are observed when light is sent through a moving medium; neutrons entering a crystal at an exact Bragg angle propagate through the crystal along the Bragg planes at a drift velocity much less than the group velocity. Ways are sought to exploit this effect. Ways are sought to use neutron interferometry to test nonlinear variants of wave mechanics. Effect of interferometer rotation; nature of coherent wave front in interferometer; single and multiple slit Fresnel diffraction patterns.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

377. MODIFICATION OF THE PROPERTIES OF BENZENE-DERIVED GRAPHITE FIBERS BY INTERCALATION AND IMPLANTATION

M. S. Dresselhaus
Center for Materials Science and Engineering
Phone: (617)-253-6864
G. F. Dresselhaus
Center for Materials Science and Engineering
Phone: (617)-253-6827

$130,000 (24 Months) 02-2

A comprehensive study of the structure and property relationships of benzene-derived fibers, both in their pristine form and as modified by intercalation and implantation. Structural, mechanical and electrical properties of these fibers approach those of graphite single crystals--superior to those of fibers formed by other techniques. Emphasis on characterization by high resolution TEM to identify defects introduced by intercalation and implantation.

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

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

$132,469 02-2

The A15 compound V_3Ga is the best known superconducting material for the fabrication of practical high field magnets. Its usefulness is, however, restricted to about 25T. This is believed to be due to the low spin-orbit scattering because of the low Z elemental components. Two approaches to increasing the spin-orbit scattering will be taken by this program--the inclusion of randomly placed high Z elements with minimum lattice distortion and thin closely spaced high Z material layers. Samples will be prepared by electron beam evaporation and characterized by the superconducting properties, resistivity and spin-polarized tunneling measurements. These measurements will test existing theoretical concepts and are expected 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.

UNIVERSITY OF MASSACHUSETTS
Amherst, MA 01003

379. ERROSION OF STRUCTURAL CERAMICS

J. E. Ritter Jr.
Dept. of Mechanical Engineering
Phone: (413)-545-0632, (413)-235-2414
K. Jakus
Dept. of Mechanical Engineering
Phone: (413)-545-2424

$38,570 (24 Months) 01-5

Erosion behavior and related strength degradation of Al_2O_3, Si_3N_4, and SiC at temperatures to 1200°C. Assessment of erosion models for predicting erosion behavior and associated strength degradation. Effect of eroding particle velocity, size, angle of impingement, temperature of environment, and subcritical crack growth on erosion rate and related strength degradation for Al_2O_3, SiC and Si_3N_4. Biaxial strength characterizations of as-prepared and eroded samples.

380. SYNTHESIS OF METASTABLE SUPERCONDUCTING COMPOUNDS BY ION IMPLANTATION AND ELECTRON BEAM MELTING AND SPIN QUENCHING

M. T. Clapp
Dept. of Mechanical Engineering
Phone: (413)-545-0868

$35,000 02-2

Ion implantation and spin quench formed metastable A-15 and amorphous superconducting materials. Ion implantation to optimize stoichiometry and to introduce selected impurities. Spin quenching used as a rapid solidification technique for amorphous materials. Furnace and electron beam annealing used to remove radiation damage in implanted samples and to crystallize amorphous preparations. Material forms: Nb_3Al, implanted with B and C; Nb_3Si and Nb_3Ge, implanted with C, N, and O.

MICHIGAN STATE UNIVERSITY
East Lansing, MI 60439

381. STUDIES ON AGE-HARDENING IN SPINODALLY MODULATED ALLOYS-EXPERIMENTAL AND THEORETICAL

K. N. Subramanian
Dept. of Metallurgy, Mechanics & Materials Science
Phone: (513)-353-5197

$60,652 01-2

Structure-property relationship and age-hardening of the spinodal alloy system Cu-10%Ni-6%Sn. Single crystal studies of mechanical properties of both one dimensionally and three dimensionally modulated alloys. Dislocation mobility studies by in-situ HVEM (with deformation stage) experiments. Application and development of elasticity and hardening theories to various multi-phase morphologies associated with the spinodal decomposition reaction. Computer analysis of the energetics of dislocation double-kink formation and for thermally activated dislocation motion. Experiments and theory concerning temperature and strain-rate dependent mechanical behavior.

MICHIGAN TECHNOLOGICAL UNIVERSITY
Houghton, MI 49931

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

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

$94,000 01-2

Hydrogen embrittlement and stress corrosion cracking with concern for the effects of (a) intergranular misorientation and segregation, (b) local chemistry variation, (c) multiaxial states of stress on such behavior. Experimental methods include (a) bicrystal studies, (b) Auger electron spectroscopy, (c) slow strain-rate testing, and (d) multiaxial deformation and fracture tests.

UNIVERSITY OF MICHIGAN
Ann Arbor, MI 48109

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

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

$92,000 01-1

Study of role and mechanism of nucleating agents on the crystallization of the Si_2N_2O containing grain 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 transmission electron microscopy, electron energy loss spectroscopy, fractography analysis.

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

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

$84,000 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.

385. 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 MINNESOTA
128 Pleasant Street, S.E.
Minneapolis, MN 55104

386. 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

$540,000 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.

387. 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

$86,369 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.

UNIVERSITY OF MINNESOTA (continued)

388. VERY LOW TEMPERATURE STUDIES OF HYPERFINE EFFECTS IN METALS

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

$78,723 02-2

Nuclei, through hyperfine coupling, used as a probe of magnetic interactions in metallic systems; emphasis on the role of conduction electrons. Nuclear singlet ground state intermetallic compounds, very dilute magnetic impurities in non-magnetic metals, and itinerant ferromagnets. Development of the sub-millikelvin refrigeration capabilities of first type and utilization in study of local moment in manganese-based Kondo systems at millikelvin and submillikelvin temperatures. The local magnetization measured with nuclear orientation and the macroscopic magnetization measured with 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

389. THEORETICAL STUDIES ON THE STRUCTURE OF INSULATING AND METALLIC GLASSES

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

$69,345 01-1

Theoretical study of atomic scale, electronic, and dynamic structure 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

390. DEVELOPMENT AND CHARACTERIZATION OF HIGH TEMPERATURE ELECTRICALLY CONDUCTING OXIDES

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

$116,000 01-3

Interrelationship of electrical conductivity, oxidation-reduction kinetics, defect structure, and composition for n type transition metal oxides TiO_2, $SrTiO_3$, and $BaTiO_3$, and p type transition metal oxides Cr_2O_3, NiO, $LaCrO_3$, and $YCrO_3$. Experimental aspects include specimens preparation, thermogravimetric measurements, x-ray diffraction, transmission electron microscopy, and ERR magnetic susceptibility, Hall, conductivity, and seebeck measurements.

391. 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.

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

H. R. Chandrasekhar
Dept. of Physics and Astronomy
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 200-100μm range.

UNIVERSITY OF MISSOURI (continued)

393. 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
J. G. Mullen
Dept. of Physics
Phone: (317)-494-3031

$175,000 (19 Months) 02-2

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

NATIONAL ACADEMY OF SCIENCES
2101 Constitution Avenue
Washington, DC 20418

394. SUPPORT OF A COMMITTEE ON MAJOR FACILITIES FOR MATERIALS SCIENCES

W. Spindel
Commission on Physical Sciences, Mathematics and Resources
Phone: (202)-334-2156

$100,000 02-2

Support for a Committee, chaired by Dr. Frederick Seitz, to establish priorities for major facilities for materials sciences, in response to a request from Dr. George Keyworth, the President's Science Advisor, and Dr. Frank Press, President of the National Academy of Sciences.

UNIVERSITY OF NEVADA
Reno, Nevada 89557

395. INVESTIGATIONS OF TRIPLET EXCITON PROCESSES OCCURRING IN PURE POLYMER FILMS

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

$80,391 03-1

Using pulsed laser excitation and luminescence monitoring in the microsecond time domain, coupled with measurement of ground state depletion, some of the fundamental photophysical rate constants associated with solid films of aromatic polymers at ambient temperature will be studied. The rate constants include those for excimer phosphorescence, radiationless deactivation of long-lived triplet excimers and triplet-triplet annihilation to form delayed excimer fluorescence. Additional investigations in the area of triplet energy transfer from terminal carbonyl groups of polystyrene chains to pendant phenyl groups. The subsequent rates of energy migration along the polymer chain will also be investigated.

NEW MEXICO INSTITUTE OF MINING & TECH.
Socorro, NM 87801

396. MICROSTRUCTURAL AND MECHANICAL PROPERTY STUDY OF SOLAR ENERGY COLLECTORS

O. T. Inal
Dept. of Metallurgical and Materials Engineering
Phone: (505)-835-5229, 5519

$95,000 (24 Months) 01-1

Effect of plating geometry, bath compositions and current densities on the surface structure of electroplated black Cr_2O_3 and anodic oxidation of leaf Zn, Zn electroplated steel, and hot-dip galvanized steel. TEM, FIM, nucleation, solar absorption, thermal cycle, mechanical adhesion studies, ZnO and Al_2O_3 film coatings, copper oxide and black nickel selective surfaces, and mathematical optimization of selective solar surfaces.

UNIVERSITY OF NEW MEXICO
Albuquerque, NM 87131

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

R. C. Ewing
Geology Dept.
Phone: (505)-277-2030

$71,500 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 a 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.

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

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

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

$93,010 01-1

Preparation of thin-film surface coatings by flow 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 synchroton radiation at the BNL NSLS.

CITY UNIVERSITY OF NEW YORK/CITY COLLEGE (continued)

399. 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.

400. MAGNETIC PROPERTIES OF DOPED SEMICONDUCTORS

M. Sarachik
Dept. of Physics
Phone: (212)-690-6924

$107,000 02-2

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

401. ELECTRONIC AND OPTICAL PROPERTIES OF DISORDERED SYSTEMS

M. Lax
Dept. of Physics
Phone: (212)-690-6864

$91,147 02-3

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

SUNY/ALBANY 518-3300 -8333 Physics
1400 Washington ave. 12222 442 B-44 4518 -8345 Corbett

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

402. RESEARCH CONSORTIUM FOR X-RAY TOPOGRAPHY 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. Acquisition of image processing equipment and development of associated software for real-time high-resolution data processing. Research includes studies of hydride precipitation in the niobium-hydrogen system, investigations 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.

403. CONSTRUCTION AND MAINTENANCE OF SUNY FACILITIES AT THE NATIONAL SYNCHROTRON LIGHT SOURCE (SEVERAL INSTITUTIONS INVOLVED)

SUNY / Albany

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

$360,000 02-2

An X-ray beam line at the National Synchrotron Light Source (NSLS) developed under the auspices of this Participating Research Team (PRT). This PRT represents campuses at Albany, Buffalo, Stony Brook, Cortland, and Alfred. Facilities and research in high resolution crystallography, surface physics, small angle scattering, and EXAFS.

404. SURFACE STUDIES: A PROPOSAL FOR A PARTICIPATING RESEARCH TEAM AT NSLS

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

$150,527 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.

246-5000 switch Board at SB

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

$100,000 03-3

A recently developed embedding theory for treating chemisorption on metals extended and applied to systems involving titanium, copper, nickel and copper/nickel alloy substrates, and H_2, H, CO, C and coabsorbed H and C adsorbates. Two of the studies, surface embrittlement of titanium by hydrogen and H_2 dissociation on a monolayer stepped copper surface are extensions of previous work. The major copper/nickel alloy project is a systematic variation of the surface composition by Cu/Ni substitution in order to probe the effect of surface composition on H and CO adsorption and the nature of the carbon-metal bond. The primary emphasis of the work is on the energetics of adsorption as a function of surface composition, with the objective of determining the reactivity of adsorbed species.

NORTH CAROLINA AGRICULTURAL & TECH. UNIVERSITY
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

$60,000 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 delamination, debonding, fiber breakage, etc. Optical and scanning electron microstructural characterization.

NORTH CAROLINA STATE UNIVERSITY
Raleigh, NC 27650

407. MICROSTRUCTURAL EFFECTS IN SOLID PARTICLE EROSION

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

$90,350 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 CENTRAL UNIVERSITY
Durham, NC 27707

408. 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

$65,843 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

409. DEVELOPMENT OF AN X-RAY BEAM LINE AT THE NSLS FOR STUDIES IN MATERIAL SCIENCE USING X-RAY ABSORPTION SPECTROSCOPY (PRT)

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

$240,000 02-2

Development of an advanced X-ray absorption fine structure (EXAFS) beam line at NSLS for a Participating Research Team (PRT) with members from North Carolina State University, University of Connecticut, University of Washington, University of Delaware, Brookhaven National Laboratory, United Technologies and General Electric. Facility for the energy range from 1-20 KeV and with provisions for EXAFS, fluorescence, and near edge spectroscopic and polarization studies. Research to be addressed: areas of metallurgy, corrosion, amorphous materials, catalysis, interfacial phenomena, electrochemistry and magnetic properties.

NORTHEASTERN UNIVERSITY
Boston, MA 02115

410. DYNAMICAL FRICTION IN CONDENSED MATTER

J. B. Sokoloff
Dept. of Physics
Phone: (617)-437-2931
C. H. Perry
Dept. of Physics
Phone: (617)-437-2913

$89,996 02-3

Joint theoretical-experimental studies of a variety of systems reflecting motion of one set of species (ions, defects, layers) relative to another set of species (channels, lattices, layers). The rate of energy dissipation, its frequency, temperature and pressure dependence will be calculated as well as electronic contributions to the damping. Experimental studies of Y_2O_3 - ZrO_2, hollandite perovskite, intercalated graphite and dichalcogenides will be related to the theoretical models, including a predicted electric field effect.

NORTHWESTERN UNIVERSITY
Evanston, IL 60201

411. 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

$175,525 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 extended to MnO and NiO. Valence in the series will be studied via X-ray absorption edge, T.E.M. critical voltage technique, and photoelectron spectroscopy. Defect interactions in MnO and CoO studied via X-ray (synchrotron) and/or pulsed neutron scattering. The self-consistent field local density theory used to calculate the electronic structure associated with isolated vacancies and defect clusters. An energy band code based on the Linearized Muffin Tin scheme used to calculate band structures, Fermi surfaces, and transport properties to correlate with the experimental studies. Theory made to more complex oxides, e.g., Fe_3O_4, $CoAl_2O_4$, and $FeAl_2O_4$.

412. FAST ION MOTION IN SELECTED VITREOUS AND CRYSTALLINE SOLID ELECTROLYTES

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

$74,946 01-1

Diffusivity of highly mobile ions in solid electrolytes which may have application in energy storage or conversion is measured using pulsed-field-gradient nuclear magnetic resonance techniques and analyzed using a dynamic bond percolation model. Specific materials to be studied include protonic-conducting crystalline beta-alumina and gallates and fast-ion conducting glasses.

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)-492-5353

$65,100 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. PRODUCTION AND STUDY OF NEW MATERIALS USING CLUSTER BEAMS

G. D. Stein
Depts. of Materials Sci. & Eng., and Mechanical & Nuclear Eng.
Phone: (312)-492-3263

$114,996 01-3

Experimental and theoretical research on: a) the development of new metal cluster sources, including binary alloy clusters, b) the comparison of cluster properties in low density molecular beams to those of the same species collected onto substrates or in matrix isolation, and c) the production of new composite materials using cluster deposition. High energy electron diffraction and laser scattering are used to study the structures and the onset of nucleation of metallic clusters as small ten atoms per cluster. These studies are carried out on clusters in-flight prior to deposition onto substrates; clusters as small as fifty atoms per cluster have been studied to date.

415. INVESTIGATION OF DEEP LEVEL DEFECTS IN EPITAXIAL SEMICONDUCTING ZINC SULPHO-SELENIDE

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

$64,395 (15 Months) 01-3

Investigation of fundamental point defect formation mechanisms in the wide bandgap semiconductor ZnSSe. Identification of deep level defects in deliberately doped and MeV electron irradiated material and exploration of their role in electrical compensation. Thermal stability of defects. Experimental techniques include optical and electrical deep level transients spectroscopy, Hall measurements, photocapacitance, and spectrally resolved photocurrent measurements.

NORTHWESTERN UNIVERSITY (continued)

416. ULTRA-LOW-TEMPERATURE NEUTRON DIFFRACTION

W. P. Halperin
Dept. of Physics and Astronomy
Phone: (312)-492-3686, 3644
J. B. Ketterson
Dept. of Physics and Astronomy
Phone: (312)-492-5468, 3644

$110,000 (24 Months) 02-1

Investigations of nuclear magnetic ordering using an ultralow temperature neutron diffraction facility at Argonne National Laboratory. Determination of the nature of the nuclear ordering in solid helium-3, a result of fundamental importance. Investigation of the ordering of nuclear spins in metals such as $PrCu_6$.

417. 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

$70,000 02-3

Determination of the thermodynamic properties and short-range order(SRO) 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 (CPA) used to obtain the density of states. These calculations to identify multi-site potentials to be used with existing theories, such as the cluster variation method of Kikuchi, to construct alloy phase diagrams.

NORTHWESTERN UNIVERSITY (Coninued)

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

$97,809 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

$84,700 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. Wilde
Dept. of Metallurgical Engineering
Phone: (614)-422-6255
D. D. Macdonald
Chemistry Lab, SRI International
Phone: (415)-859-3195

$75,000 01-1

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

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

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

$65,992 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.

422. FUNDAMENTAL STUDIES OF HIGH TEMPERATURE CORROSION REACTIONS

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

$99,950 01-3

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.

OHIO STATE UNIVERSITY (continued)

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

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

$111,245 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

PENNSYLVANIA STATE UNIVERSITY
University Park, PA 16802

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

M. W. Grutzeck
Materials Research Laboratory
Phone: (814)-865-3539

$59,817 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 fo 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)

425. VIBRATIONAL AND OPTICAL STUDIES OF AMORPHOUS METALS

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

$82,800 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 dielectric layer and reflecting layer to produce a minimum in the reflectance and thus reduce the background light when measuring the Raman scattered light. The study is initially focussed 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.

426. SPECTROSCOPIC INVESTIGATIONS OF GLASS STRUCTURE

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

$116,881 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 infared 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 metals in high magnesium content glasses.

427. GRAIN BOUNDARY AND SURFACE DIFFUSION IN OXIDE SYSTEMS

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

$54,800 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)

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

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

$64,516 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.

429. MECHANISMS OF WEAR IN SINGLE AND TWO PHASE MATERIALS

N. H. Macmillan
Materials Research Laboratory
Phone: (814)-863-0180

$96,200 01-5

Experimental comparison of the resistance of various classes of materials to solid particle erosion, slurry erosion, and rolling-tumbling-sliding wear by angular WC-Co particles; specimen preparation by powder methods; study of particle trajectories and impact parameters by cinematography; characterization of wear by optical and electron microscopy, weight loss measurements and surface profilometry. Materials systems to include (i) brittle ($PbO-B_2O_3-SiO_2$ glass, Al_2O_3) and ductile (Pb,Cu) single phase and (ii) brittle-brittle (Al_2O_3 in $PbO-B_2O_3-SiO_2$ glass), brittle-ductile (Al_2O_3 in Pb), ductile-brittle (Cu in $PbO-B_2O_3-SiO_2$ glass) and ductile-ductile diphasic materials.

430. 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.

PENNSYLVANIA STATE UNIVERSITY (continued)

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

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

$88,000 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.

UNIVERSITY OF PENNSYLVANIA
Philadelphia, PA 19104

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

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

$79,973 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.

David White x 8571

UNIVERSITY OF PENNSYLVANIA (continued)

433. LOW STRESS BRITTLE FRACTURE IN POLYMERS

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

$81,500 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.

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

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

$106,000 01-2

Identification of microsctructural 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)

435. INTRINSIC SURFACE PHONONS ON RECONSTRUCTED SEMICONDUCTOR SURFACES

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

$104,216 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.

436. HIGH CONDUCTIVITY PROTON SOLID ELECTROLYTES

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

$103,127 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^+- 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

437. HIGH TEMPERATURE CORROSION OF CERAMICS

F. S. Pettit
Dept. of Metallurgical and Materials Engineering
Phone: (412)-624-5300
J. R. Blachere
Dept. of Metallurgical and Materials Engineering
Phone: (412)-624-5296

$65,000 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, sulfidizing, 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.

UNIVERSITY OF PITTSBURGH (continued)

438. 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.

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

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

R. D. Parks
Dept. of Physics
Phone: (212)-643-2071

$90,000 02-2

Photoemission studies of rare earth and early actinide systems with the aim of understanding the electronic phenomena underlying the 4f-instabilities in mixed valent and Kondo lattice systems and narrow 5f-band behavior in the early actinides. XPS studies performed at Polytechnic and synchrotron-radiation-stimulated photoemission studies at NSLS.

440. 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.

POLYTECHNIC INSTITUTE OF NEW YORK (continued)

441. 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.

PRINCETON UNIVERSITY
Princeton, NJ 08544

442. 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

$80,000 03-1

A program is proposed to examine the fundamental relationship between chain conformational changes and resultant macroscopic material responses during deformation. The program is based on the coupling of rheological and rheo-optical measurements during deformation. An in situ infrared dichroism technique is described by which molecular orientation may be characterized dynamically during polymer deformation and relaxation. The use of novel specimens that are partially deuterium labelled allows characterization of local chain segment orientation. The information is not obtainable by present techniques and is of sufficient detail to allow a test of current theories of polymer chain relaxation by reputational motion. The information is of importance in understanding the relationship between polymer processing conditions and polymer material behavior.

PRINCETON UNIVERSITY (continued)

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

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

$85,000 03-1

Research is proposed 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. Included is research of the process of electron ejection into the lattice by studying the phototransfer of electrons from a set of donor ions to a set of 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

444. NOVEL POLYMERIC Li AND DIVALENT CATION FAST ION CONDUCTING MATERIALS: LI-SALT-IONENIC POLYMER SOLUTIONS, LI CONTAINING PLASTIC CRYSTAL PHASES AND MI_2-$M(PO_3)_2M(PS_3)_2$ GLASSES

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

$82,782 01-1

Preparation and characterization of novel fast ion conductors. Formation of a unique type of "molten salt" systems by dissolution of lithium salts in salts of quaternary nitrogen cations in eight polymeric or related structure forms. Studies of Li^+-ion conduction mechanisms. 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-$M(PO_3)_2M(PS_3)_2$, where M^{2+} is Pb^{2+}, Cd^{2+}. Characterizations include measurements of electrical conductivity, nuclear magnetic resonance, viscoelastic properties, and glass transition temperatures.

PURDUE UNIVERSITY (continued)

445. 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

$480,000 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.

446. MECHANISMS OF ELEVATED TEMPERATURE RUPTURE IN SINGLE PHASE CERAMICS

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

$93,000 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 (a) tensile creep using constant true stress, (b) 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 and carbonyl Ni.

PURDUE UNIVERSITY (continued)

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

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

$87,917 01-3

The objectives are (a) 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; (b) to characterize the ZFP compositions in terms of diffusion paths and thermodynamic data; (c) to study the feasibility of regulating the interdiffusion of elements with preferential development of ZFP's. ZFP's for individual components within the diffusion zone of either a single or multiphase multicomponent have been identified. At ZFP's the interdiffusion flux of a given component goes to zero and exhibits reversal in its flow direction on either side of the plane.

448. 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

$89,119 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 the 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)

449. 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

450. TESTS AND MODELING FOR SINTERING THEORY

R. H. Doremus
Dept. of Materials Engineering
Phone: (518)-266-6709
R. M. German
Dept. of Materials Engineering
Phone: (518)-266-6445

$85,000 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 adsorption.

451. EFFECT OF WELDING VARIABLES ON THE SOLIDIFICATION SUBSTRUCTURE, MECHANICAL PROPERTIES & CORROSION BEHAVIOR OF STAINLESS STEEL

W. F. Savage
Materials Division
Phone: (518)-266-6780
D. J. Duquette
Materials Division
Phone: (518)-266-6490

$141,875 01-1

Corrosion of ferritic steel weldments in aqueous chloride environments; and the effect of welding parameters; effect of delta ferrite on localized corrosion; Cr depletion at grain boundaries; synergistic effect of sulfate and chloride ions on initiation and propagation of stress corrosion cracks; role of grain boundary precipitation; role of surface films; weldability and hot cracking of ferritic steels.

RENSSELAER POLYTECHNIC INSTITUTE (continued)

452. OXIDATION MECHANISMS IN METALS

R. K. MacCrone
Dept. of Materials Engineering
Phone: (518)-266-6047

$80,000 01-3

Study of both point defects, impurities, and grain boundaries in films of the metal oxides NiO, WO_2. Techniques include both discontinuous and continuous thermogravimetric analysis, electron paramagnetic resonance, Raman spectroscopy, TEM, static magnetization, and two point electrical conductivity for the purpose of obtaining a more precise understanding of the oxidation process.

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

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

$145,704 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. Non-traditional optical techniques developed and exploited: Raman spectroscopy, reflectance and ellipsometry, photovoltage spectroscopy, infrared emission, and X-ray absorption fine structure.

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

454. PROPERTIES OF MOLECULAR SOLIDS AT HIGH PRESSURE AND TEMPERATURE

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

$66,773 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

455. 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

$54,955 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).

456. 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

$185,000 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

457. 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.

458. DIFFUSIONAL CREEP OF MULTICOMPONENT SYSTEMS

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

$90,994 01-2

Research on stress-motivated diffusion in amorphous and crystalline materials, and elastic plastic deformation in oxide glasses and ceramic, polymeric, and metallic materials. The techniques of "impression" creep, fatigue, load-relaxation and elastic deformation are employed, which utilize very localized loads, and enable determination of localized load-deformation relationships that are representative of bulk behavior. Specific activities include investigations of charged dislocations in KCl, dislocation-crack tip interactions and the density of mobile dislocations.

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

459. FABRICATION SCIENCE OF SILICON NITRIDE MATERIALS

F. F. Lange
Phone: (805)-498-4545
P. E. D. Morgan
Phone: (805)-498-4545

$203,681 01-1

Evaluation of the influence of new colloidal precipitation and conventional powder preparation methods for the preparation of Si_3N_4 powder on the microstructure and microchemistry of both green and sintered compacts. Development of a colloidal method for preparing Si_3N_4 synthesis materials by investigating the slip casting of colloidally mixed slips. Study of the Si-S-N chemistry for the synthesis of Si_3N_4 powder. Techniques to obtain a homogeneous distribution of sintering aids and their effect on the resultant microstructure and microchemistry. Development of quantitative methods based on X-ray microanalysis and backscattered electron imaging, for gauging compositional uniformity of powder compacts and sintered materials.

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

460. LOCAL STRUCTURE OF METAL ATOMS IN SILICA AND SILICATES

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

$70,092 01-3

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

RUTGERS UNIVERSITY (continued)

461. 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

$130,000 02-2

Develop high pressure diamond anvil cell for electron paramagnetic resonance measurements. Study of phase transitions in phosphorus doped silicon, organic charge transfer salts, europium compounds and cesium using this apparatus.

SRI INTERNATIONAL
Menlo Park, CA 94025

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

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

$114,457 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.

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

$67,522 03-3

The single turnover reaction sequence recently developed for the surface characterization of Pt/CPG catalysts will be expanded as a means of characterizing other catalysts and support combinations. With the availability of these characterized catalysts and the development of a means to prepare catalysts having specific site densities, these catalysts can be used in the study of a variety of catalytic reactions to correlate with those taking place on well characterized surfaces of metallic single crystals and to provide information of value in the preparation of selective and efficient catalysts, for a variety of catalytic processes.

UNIVERSITY OF SOUTHERN CALIFORNIA
Los Angeles, CA 90089-0241

464. GRAIN BOUNDARY SLIDING AND DEFORMATION MECHANISMS DURING HIGH TEMPERATURE CREEP

T. G. Langdon
Dept. of Materials Science and Mechanical Engineering
Phone: (213)-743-2095

$40,400 (4 Months) 01-2

Measurements of creep and grain boundary sliding in Al and Mg-based alloys stress and temperature dependences; threshold creep stress in precipitation hardened and solid solution strengthened Al-base alloys; boundary migration and sliding in cyclic creep; cavitation in Cu and Cu alloys.

465. ELECTRICAL AND MECHANICAL PROPERTIES OF OXIDE CERAMICS

F. A. Kröger
Dept. of Materials Science
Phone: (213)-743-6224

$90,000 01-3

Relationship between the composition and microstructure with physical behavior of oxide ceramics, principally Al_2O_3. Relationship of composition, including non-stoichiometry, and microstructure to dopants, conditions of preparation, oxygen fugacity, and temperature, and their effect on physical properties through the defect structure. Experimental studies include electrical conductivity, emf measurements on concentration cells to determine partial ionic and electrical conductivities, electron-spin resonance, optical absorption, and creep.

UNIVERSITY OF SOUTHERN CALIFORNIA (continued)

466. 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

$130,031 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.

SOUTHERN ILLINOIS UNIVERSITY
Carbondale, IL 62901

467. METALLIC GLASSES AS NEW CATALYST SYSTEMS FOR ENERGY CONVERSION

G. V. Smith
Molecular Science Program and Department of Chemistry
Phone: (618)-453-2785,(618)-453-572
W. E. Brower Jr.
Dept. of Mechanical Engineering and Materials
Phone: (618)-536-2396

$40,040 01-1

Selectivity of glassy metallic catalysts related to structure of amorphous metal surfaces and stability of amorphous and nonequilibrium crystalline surface features. Materials studied - Pd-Si, Fe-B, and Zr-Ni alloys prepared by rapid solidification via modified shock tube, hammer and anvil, and single roller techniques. Use of (+)-apopinene as molecular probe for characterizing metallic glasses by correlating with surface features the ratio of isomerization to addition during hydrogenation. Analysis of surface structure with ESCA, ISS, BET surface area, and chemisorption techniques, and of bulk structure with XRD, Mössbauer spectroscopy, TEM, and thermal analyses methods.

SOUTHWEST RESEARCH INSTITUTE
6220 Culebra Road
San Antonio, TX 78284

468. CHARACTERIZATION OF PORE EVOLUTION IN CERAMICS DURING CREEP FAILURE AND DENSIFICATION

R. A. Page
Dept. of Materials Science
Phone: (512)-684-5111 X3252
J. Lankford
Dept. of Materials Science
Phone: (512)-684-5111 X2317

$160,084 01-2

Characterization and modeling of cavity nucleation and growth during creep of ceramics using small-angle neutron scattering (SANS), density measurements, transmission electron microscopy (TEM), and Auger electron microscopy. SANS and TEM analysis of pore removal during sintering. Materials under investigation are Al_2O_3, SiC, and Si_3N_4.

STANFORD UNIVERSITY
Stanford, CA 94305

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

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

$210,000 01-2

Development of a new unified computer model for elevated-temperature fatigue that is based upon explicit representations of the controlling internal physical processes. 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. Research advances earlier modelling work (the development of MATMOD and MATCON constitutive relations) on the plasticity of materials.

STANFORD UNIVERSITY (continued)

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

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

$85,000 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.

471. PHOTOELECTRONIC PROPERTIES OF II-VI HETEROJUNCTIONS

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

$197,000 01-3

Interactions occurring at the interface between CdTe with other materials, and the role of interfacial microstructure and microchemistry on the electrical properties of such CdTe containing heterojunctions. Effects of etching and heat treatment on surfaces, Schottky barriers, and heterojunctions formed on CdTe, and the preparation and behavior of polycrystalline films of CdTe. Grain boundary characterization and passivation. Measurements include J-V curves in dark and light; junction capacitance; surface photovoltage; Schottky-barrier formation; spectral response; and diffusion lengths. Scanning transmission electron microscopy and high resolution TEM analysis of heterojunction interfaces; lattice resolution; electron microdiffraction; XPS, Auger analysis; vacuum evaporation; spray pyrolysis; rf sputter deposition, magnetron sputtering, and chemical vapor deposition, and closed-space vapor transport techniques.

472. EVALUATION OF MACHINING DAMAGE IN BRITTLE MATERIALS

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

$94,285 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)

473. THE USE OF SURFACE ACOUSTIC WAVES TO STUDY SMALL FATIGUE CRACKS

D. V. Nelson
Dept. of Mechanical 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

474. STUDIES OF MAGNETISM AND EXCHANGE SCATTERING IN SOLIDS USING SYNCHROTRON RADIATION AND SPIN POLARIZED PHOTOELECTRONS

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

$139,000 02-2

A synchrotron light source will be used to produce polarized photoelectrons from transition metal ions. The multiplet splitting serves as the polarizer. Spin polarized EXAFS will be used to study instantaneous short range magnetic order above and below transition temperatures and on surfaces and to study temperature dependence of short range order above transition temperatures.

SYRACUSE UNIVERSITY
Syracuse, NY 13210

475. THE CATALYTIC REACTIVITY TO THIN FILM CRYSTAL SURFACES

R. W. Vook
Dept. of Chemical Engineering and Materials Science
Phone: (315)-423-3466
J. A. Schwarz
Dept. of Chemical Engineering and Materials Science
Phone: (315)-423-4575

$150,000 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

476. STATISTICAL MECHANICS OF POLYMER SYSTEMS

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

$82,354 03-1

A theoretical investigation into the equilibrium and dynamic behavior of amorphous polymers over a broad range of concentration, molecular weight, and temperature. The investigations involve non-equilibrium thermodynamics, equilibrium and non-equilibrium statistical mechanics, and computer simulation. Specific problems include more realistic models for single chain dynamics, conformation and dynamics of chains in semidilute and bulk systems and equilibrium and dynamic aspects of the glass transition.

UNIVERSITY OF TEXAS
Austin, TX 78712

477. 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

$115,000 02-2

Photoemission from electrodes into dielectric fluids and time of charge transport studied 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

478. 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)-581-3589, 4850, 6863

$80,000 01-1

Systematic investigation of the electron 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 APS datta with existing LCAO, cluster model, and self-consistent linear muffin tin LMT band-structure calculations.

UNIVERSITY OF UTAH (continued)

479. FABRICATION, PHASE TRANSFORMATION STUDIES AND CHARACTERIZATION OF SiC-AlN-Al_2OC

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

$99,181 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 equilibria, precipitate morphology, spinodal decompositions and grain boundaries especially with special regard to the nucleation and growth of possible grain boundary phases. Evaluation of room temperature bend strength and fracture toughness and elevated temperature creep. Emphasis on understanding the inter-relationship of fabrication, microstructure, and mechanical behavior.

480. 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

$78,083 01-3

Development of an understanding of miscibility gaps in alloys including organometallic vapor phase epitaxy growth of metastable alloys, the effect of short range (100Å to 1000Å) clustering or 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.

VIRGINIA POLYTECHNIC INST. & STATE UNIV.
Blacksburg, VA 24061

481. FRACTURE MECHANISMS IN GLASS-CRYSTAL COMPOSITES

D. P. H. Hasselman
Dept. of Materials Engineering
Phone: (703)-961-5402

$77,000 01-2

Fracture mechanisms in glass-crystal composites with a cordierite glass-ceramic and its original (non-crystallized) glass, glass-alumina composites, and Richterite glass ceramics as the principal materials of study. Flaw introduction by micro-hardness indentation and crack characterization by scanning electron microscopy. Characterization of localized stress distribution near crystalline dispersions, sub-critical and critical crack propagation behavior, associated crack-crystalline interaction, and mechanisms which control the nature (size, geometry) of the fracture-initiating flaw. Biaxial flexure and double torsion of double cantilever beam strength characterizations. Environmental and loading conditions include ambient room air and inert environments, and variable loading rates to establish strain-rate sensitivity.

UNIVERSITY OF VIRGINIA
Charlottesville, VA 22901

482. THE EFFECT OF MICROSTRUCTURE ON THE FATIGUE BEHAVIOR OF FE-C-X ALLOYS

G. J. Shiflet
Materials Science Department
Phone: (804)-924-6340
E. A. Starke Jr.
Materials Science Department
Phone: (804)-924-7097

$60,000 (15 Months) 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.

UNIVERSITY OF VIRGINIA (continued)

483. SPECTROSCOPY OF SURFACE ADSORBED MOLECULES

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

$104,377 02-2

Investigations of the properties of surfaces and interfaces containing molecular adsorbates using elastic electron tunneling spectroscopy (IETS), photoemission (ESCA), and Auger spectrocopies. IETS studies of combinations of oxide substrate and metal overlayer electrodes to establish the nature of the chemical and electronic interactions between molecules and interface: ESCA and Auger studies to augment the IETS work. Studies of UV-induced damage to molecules and photocatalytic effects on semiconductor oxides.

484. MAGNETIC IMPURITIES IN SUPERCONDUCTORS

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

$92,423 02-3

Theoretical research on magnetic impurity interactions in superconductors. 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 impurities, at intermediate concentrations, on the electron spin susceptibility and nuclear spin relaxation rate. Emphasis on new mechanisms for achieving enhancement of superconducting properties in high magnetic fields.

WASHINGTON UNIVERSITY
St. Louis, Missouri 63130

485. 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

486. NUCLEAR MAGNETIC RESONANCE STUDIES OF LOW MOTION IN FAST ION CONDUCTING SOLIDS

J. L. Bjorkstam
Dept. of Electrical Engineering
Phone: (206)-543-2177

$91,720 01-3

Nuclear magnetic resonance (NMR) studies of fundamental ion transport processes in fast ion conducting crystals and glasses. Measurements of ion dynamics and ion-lattice dynamics in beta aluminas, lithium ion conductors, and borophosphate glasses, and of ion leaching in glasses. The program includes modeling of correlation functions for ion transport in solids and development of improved microprocessor-based NMR instrumentation.

487. X-RAY SPECTROSCOPY OF SOLIDS UNDER PRESSURE

R. L. Ingalls
Dept. of Physics
Phone: (206)-543-2778

$78,000 02-2

Structure and behavior of materials at high pressure by pressure-sensitive phase transformations. The X-ray absorption near-edge structure (XANES) on materials exhibiting structural or thermal disorder-liquid metals and layered compounds.

488. FUNDAMENTAL STUDIES OF ELASTOMERS

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

$105,948 03-1

Research to synthesize and characterize elastomers cross-linked by the formation of metal-chelate bonds. Elastomers useful for the determination of the strain dependence of the junction pair correlation function are the primary focus. Theoretical studies tc understand network formation processes. Computer simulations of gelation to determine scaling laws for various types of cross-linking systems.

UNIVERSITY OF WEST VIRGINIA
Morgantown, WV 26506

489. ELECTRON HYBRIDIZATION EFFECTS AND THE CRYSTAL STRUCTURE OF PLUTONIUM

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

$62,351 03-1

Theoretical studies of the crystallographic allotropic transformations of elemental plutonium. Band calculations of the electronic structure, lattice energy, and correlation effects for plutonium and plutonium compounds.

UNIVERSITY OF WISCONSIN
Madison, WI 53706

490. ANALYSIS OF MICROPHASE SEPARATION IN ION CONTAINING POLYMERS

S. L. Cooper
Dept. of Chemical Engineering
Phone: (508)-262-1092

$233,050 (24 Months) 03-1

Investigations of the microstructure of several ionomer systems using techniques which probe different aspects of the structure. Development of a unified model of the morphology which can rationalize the unique physical properties of these materials. Of special interest, the Nafion® ionomers because of their applications in electrochemical processes as selectively permeable membranes. The local arrangement of atoms in the ionic domains studied using Extended X-ray Absorption Fine Structure (EXAFS) analysis and XANES spectroscopy. Information about larger scale structure obtained from X-ray scattering and transmission electron microscopy experiments. To better understand the reason for differences between various ion containing polymers, the effects of several composition and preparation variables explored.

UNIVERSITY OF WISCONSIN (continued)

491. THE STABILITY OF AMORPHOUS METALS ON SEMICONDUCTOR SUBSTRATES

J. D. Wiley
Dept. of Electrical and Computer Engineering
Phone: (608)-263-2354, 1643
J. H. Perepezko
Dept. of Metallurgy and Mineral Engineering
Phone: (608)-263-1678

$84,470 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 mechanisms, and film/substrate interdiffusion at temperatures near the glass-transition temperature by structural, calorimetric, and electrical measurements. Examination of structural relaxation by electrical resistivity measurements during post-deposition annealing. Measurement of diffusion and interdiffusion by a combination of Rutherford backscattering 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.

492. OPTICAL STUDIES OF DYNAMICAL PROCESSES IN DISORDERED MATERIALS

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

$95,706 02-2

A comprehensive study of relaxation and energy transfer properties of optically-active disordered systems and exploratory investigations of doped ceramics. A capability to measure coherent 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 a prototypical glass system.

UNIVERSITY OF WISCONSIN (continued)

493. SURFACE EXCITATIONS AND THEIR INTERACTION WITH LOW ENERGY ELECTRONS

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

$87,000 02-2

Theory of electron energy loss spectroscopy (EELS) and other inelastic scattering at surfaces. Vibrational properties of isolated adatoms and ordered overlayers on metal surfaces, with emphasis on quantitative comparisons with experiment. Role of image potential in large-angle EELS and in LEED studies. Large-angle inelastic scattering from substrate phonons. EELS spectral densities at large wave vector. Surface relaxation, anharmonicity, and surface lattice dynamics. This program coupled to that of D. L. Mills, University of California-Irvine.

XEROX PALO ALTO RESEARCH CENTER
3333 Coyote Hill Road
Palo Alto, CA 94304

494. SEVENTEENTH INTERNATIONAL CONFERENCE ON THE PHYSICS OF SEMICONDUCTORS

R. Z. Bachrach
Phone: (415)-494-4157

$20,000 (24 Months) 02-2

Partial support for the Seventeenth International Conference of Semiconductors, an IUPAP biannual meeting, held August 5-10, 1984 in San Francisco. Some major topics: Electronic States, Impurity States, Excitons, Polaritons, Electron-Hole Liquid and Plasmas, Transport, Recombination, Lattice Dynamics, Low Dimensional Materials, Superlattices and Quantum Wells, Amorphous Semiconductors, and Optical Characteristics. About one thousand to attend.

NATIONAL BUREAU OF STANDARDS
Washington, DC 20234

495. INTERAGENCY PROGRAM FOR SUPPORT OF CRITICAL DATA COMPILATIONS

D. R. Lide - Office of Standard Reference Data
Phone: (301)-921-2467

$200,000

Support for the critical evaluation of data in the physical sciences and for the preparation of compilations of standard reference data is being provided through a collaborative program involving the National Bureau of Standards, National Science Foundation, Office of Naval Research, and the Department of Energy. Thermodynamic and phase equilibria data evaluation and compilation represent the principal thrust of this program.

OAK RIDGE ASSOCIATED UNIVERSITIES
P. O. Box 117
Oak Ridge, TN 37831-0117

A. Wohlpart - Phone (FTS) 626-3421 or (615) 576-3421

496. DOE FACILITY USERS PROGRAM
A. Wohlpart

$140,000 01-1

Collaborative research between university, industry, and national laboratory scientists in materials sciences to foster access to and use of advanced facilities. The SHaRE (Shared Research Equipment Program) facility includes state-of-the-art capabilities in the areas of transmission and analytical electron microscopy, surface analysis, and nuclear microanalysis; approximately 20% of the usage of these facilities is by SHaRE users for basic and applied research on energy-related materials problems, based on research proposals approved by a review committee. The ORSOAR (Oak Ridge Synchrotron Organization for Advanced Research) program involves the National Synchrotron Light Source at the Brookhaven National Laboratory to study the structures of a wide variety of amorphous and crystalline materials including metallic glasses and liquids containing more than one element, heterogeneous catalysts, surface structures, corrosion films, defects and deformed materials, and local atomic arrangements in metal alloys and ceramics; approximately 40% of the beam time will be allocated to users based on a proposal basis.

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.

JUPITER INTERNATIONAL
919 East State Street
Ithaca, NY 14850

501. SUPERPLASTIC - FORGING OF STRUCTURAL CERAMICS

Prakash Panda
Staff Scientist
Phone: (607)-273-6054

$50,000 (6 Months) SBIR

To ascertain the feasibility of superplastic forming of engineering ceramic materials, namely, silicon nitride, and glass-ceramic/silicon-carbide-fibre composites. Work will be extended to other candidate materials such as silicon-carbide, zirconia, alumina, spinels and other ceramic-ceramic composites, and CAD/CAM techniques developed and applied to superplastic forming of structural ceramics.

MICROMATERIALS TECHNOLOGY
634 South Main Street
Athens, PA 18810

502. RAPIDLY SOLIDIFIED, SPHERICAL, FINE CERAMIC POWDERS

Richard F. Cheney
Technical Director
Phone: (717)-888-6505

$49,670 (6 Months) SBIR

Determination of the feasibility of making rapidly solidified ceramic powders which are spherical and less than 3 micrometers in average diameter. Rapid solidification technology has been applied to metals with significant improvements in electrical, mechanical, corrosion and wear resistant properties. It is expected that equally significant improvements will be found for ceramics. Properties of the new powders will be evaluated and their densification behavior will be determined using press/sinter and hot-pressing techniques. The properties of selected densified parts will be evaluated.

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

503. PROCESSING AND CHARACTERIZATION OF SILICON CARBIDE-ALUMINUM OXYCARBIDE CERAMICS

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

$49,985 (6 Months) SBIR

To characterize the microstructure and mechanical properties of the sinterable SiC-Al_2OC materials to determine if they are candidates for use in the heat engines, cutting tools, wear parts and other high temperature components. Focus on two methods of synthesizing the desired solid solutions and optimization of processing and composition an important aspect of the study. X-ray diffraction, transmission electron microscopy and energy dispersive spectroscopy used to confirm the existence of a solid solution in the pressureless sintered materials and look at the grain boundary chemistry. Room temperature fracture toughness, hardness, flexural strength and high temperature creep experiments to establish baseline properties and determine the utility of using this new material in high temperature appplications. It is anticipated that SiC-Al_2OC can replace metal bonded carbides (i.e. WC-Co) in some cutting tool applications and thereby reduce the U.S. dependence on cobalt, a strategic metal.

GORHAM INTERNATIONAL
209 Mosher Road
South Windham, ME 04038

504. CONTAINERLESS SINTER/HOT ISOSTATIC PRESSING (HIP) OF A SIALON

Andrew C. Nyce
Materials, Energy and Environmental Division
Phone: (207)-892-2216

$49,993 (6 Months) SBIR

Study is to determine the feasibility of fully densifying a SiAlON via sinter/HIP processing. In this process technology investigation, green preforms are sintered under moderate N_2 pressure to high density and closed porosity in the HIP vessel; following completion of the designated sintering phase of the cycle, the vessel is rapidly pressurized to a suitable HIPing pressure (e.g., 30 KPSI), and the HIP phase of the cycle is then conducted. Sinter/HIP expected to yield technically unique materials with properties and microstructures unlike those produced via other process technologies. The work will aim at fully densifying a 92 wt.% Si_3N_4 + 6 wt.% Y_2O_3 + 2 wt.% Al_2O_3 SiAlON via sinter/HIP. Room temperature modulus of rupture values for sinter/HIPed specimens generated and compared with MOR values for compositionally similar sintered and sintered + containerless HIPed specimens.

KJS ASSOCIATES
1616 Hillrose Place
Fairborn, OH 45342

505. EVALUATION OF METAL-MATRIX COMPOSITES BASED ON FE-ND-3 ALLOYS FOR IMPROVED PERMANENT MAGNETS

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

$49,500 (6 Months) SBIR

Heat-bonded composites of hard magnetic alloy powders in a ductile metal matrix fabricated and characterized for potential high energy permanent magnet applications. The applicability of Sn/Pb-solder bonding to iron-neodymium-boron alloys experimentally explored. Powders of different particle sizes prepared from pre-sintered Fe-Nd-B, compacts of these with solder powder additions made and heat-bonded by immersion in a solder bath. The quality at the bond studied metallographically and by compression tests. Magnetic properties and the composite stability at environmental temperatures up to 150°C. Aging behavior compared with that of sintered Fe-Nd-B and $SmCo_5$, and with polymer and solder-matrix magnets made from Sm-Co and other rare earth-transition metal alloys.

MARKO MATERIALS INC.
144 Rangeway Road
North Billerica, MA 01862

506. RAPIDLY SOLIDIFIED MAGNETIC ALLOYS FOR HIGH FREQUENCY, HIGH POWER APPLICATIONS

Ranjan Ray
President
Phone: (617)-663-2210

$50,000 (6 Months) SBIR

Metallic glasses fill a magnetic materials gap between nickel-iron soft magnetic alloys (the permalloys) and soft ferrites; show outstanding promise as a low loss, high-magnetic-induction core materials for the growing high-frequency, high-power applications markets. While hysteretic losses are known to originate from magnetoelastic interactions, the exact mode of coupling is not known. A model of the coupling is proposed which, if proven to be correct, should aid in designing transformer cores of lower loss. A series of measurements will be carried out to determine whether to avoid these losses through use of a non-magnetostrictive, cobalt-base glass or through more careful heat treatment of the higher induction but magnetostrictive iron-base amorphous alloys.

TECHNICAL RESEARCH ASSOCIATES INC.
410 Chipeta Way, Suite 222
Salt Lake City, UT 84108

507. OXIDE DISPERSION STRENGTHENED (ODS) TUNGSTEN CARBIDE-COBALT

Guy B. Alexander
Senior Vice President
Phone: (801)-582-8080

$49,718 (6 Months) SBIR

Cobalt is a strategically important element, and minimizing its use is a problem of national significance. Cobalt is used in cemented carbides, particularly tungsten carbide-cobalt, which are in turn used for metal cutting, mining tools, wire drawing dies and the like. In this program, a novel way to improve the properties of WC-Co alloys, and thus improve the use life of such alloys in cutting tools, mining tools, etc. will be investigated. WC-Co alloys of higher hardness at a fixed rupture strength and/or higher strength at fixed hardness and the use life of such new materials will be grossly improved. These improvements will occur because the tungsten carbide will be slightly finer grained than in conventional alloys, carbon content will be very tightly controlled, and the cobalt will be oxide dispersion strengthened.

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

$49,873 (6 Months) SBIR

An investigation using eddy current nondestructive evaluation (NDE) techniques to achieve control of surface layers and to identify defects in surface regions modified in terms of microstructure and/or composition with laser heating. The target: establish a suitable laser glazing model, determine the applicability of eddy current NDE techniques, measure properties of laser glazed layers in known alloys and in cast iron and high speed steels of interest in energy-related industries, and optimize the system parameters. This will facilitate the controlled fabrication of quality amorphous films that exhibit superior properties with respect to corrosion and strength.

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.

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

511. 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 objectives: 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

512. 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

$142,510 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 edge-supported pulling (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 (HESP) method for the production of silicon crystals.

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

513. 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.

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

$233,333 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

$249,990 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

Collaborative Research Centers

Basic materials research which is long range, generic in nature is supported by the Office of Basic Energy Sciences/Division of Materials Sciences to provide an underpinning for the development of energy technologies. In the pursuit of this research goal, facilities or centers have been and are being developed which are unique and/or expensive and costly to reproduce. Scientists from other laboratories outside of the host laboratory are encouraged to make use of these unique facilities. In this section, a description is included for most of the important centers together with a statement of the method of gaining access to them. Collaborations carried out by outside users have to be in the furtherance of DOE objectives. Any activity which can be carried out through commercially available laboratories is not appropriate for these DOE centers. Proprietary research cannot be conducted unless there is full cost recovery. Each center has a slightly different mode of operation tailored to its best use. For more information, please contact the laboratory personnel listed.

NATIONAL SYNCHROTRON LIGHT SOURCE

Brookhaven National Laboratory
Upton, New York 11973

The National Synchrotron Light Source (NSLS) facility consists of a 750 MeV (9 electron bunch) storage ring for VUV and IR research and a 2.5 GeV (30 electron bunch) 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 will be 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 are being 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.

General Users will be able to perform experiments on an NSLS facility beam line or on a PRT beam line which will be 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 will 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 Light Source.

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 NSLS or at the HFBR. It is aimed at university users having only limited grant support for their research, and will be used to support only the most deserving cases.

PERSON TO CONTACT FOR INFORMATION

R. Klaffky
NSLS - Bldg. 510E
Brookhaven National Laboratory
Upton, New York 11973

(516) 282-4974
(FTS) 666-4974

NATIONAL SYNCHROTRON LIGHT SOURCE

TECHNICAL DATA

Facilities	Key Features	Operating Characteristics
VUV electron storage ring	high brightness, continuous wavelengh 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
Superconducting wiggler	$\lambda > .1$ Å; high intensity
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 ($\lambda > 4$ Å). 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

The HFBR serves the U.S. scientific community and there exists a strong collaboration between the Brookhaven staff and users from universities, industry, and other national laboratories. In 1982 more than 160 persons from outside institutions participated in experiments at Brookhaven. Experiments are scheduled at the HFBR following review of research proposals. Please contact R. Klaffky for more information and for a copy of the HFBR Handbook which contains considerable detail on the available equipment and on operating procedures.

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

R. Klaffky
NSLS - Bldg. 510E
Brookhaven National Laboratory
Upton, New York 11973

(516) 282-4974
FTS 666-4974

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: $0.03 < Q < 10 \text{Å}^{-1}$
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 37830

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 sec, and the flux at the inner end of the beam tubes is slightly greater than 10^{15} neutrons/cm^2 sec. A wide variety of neutron scattering instruments have been constructed with the support of the Division of Materials Sciences. Three of these are unique within this country: the double-crystal small-angle diffractometer, the correlation chopper, and the wide-angle time-slicing diffractometer.

USER MODE

These facilities are open for use by outside scientists on problems of high scientific merit. Written proposals are reviewed for scientific feasibility by an internal 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 are available on request.

PERSON TO CONTACT FOR INFORMATION

H. A. Mook
Solid State Division
Oak Ridge National Laboratory
Post Office Box X
Oak Ridge, Tennessee 37830

(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 - 2.6×10^6 neut/cm^2 sec 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 Å Beam size - 5 by 3.7 cm max. Flux - 9×10^6 neut/cm^2 sec at sample with 40' collimation
HB-2A	Liquid diffractometer with linear position sensitive detector	Beam size - 1 by 3.4 cm max. λ = 0.89 Å Flux - 6.8×10^5 neut/cm^2 sec at sample with 20' collimation
HB-2, HB-3	Triple-axis, variable E_o	Beam size - 5 by 3.7 cm max. Flux - 10^7 neut/cm^2 sec at sample with 40' collimation
HB-3A	Double-crystal small-angle diffractometer	Beam size - 4 x 2 cm max. Flux - 10^4 neut/cm^2 sec λ = 2.6 Å Resolution - 4×10^{-5} Å^{-1}
HB-4A	Four-circle diffractometer	Beam size - 5 x 5 mm Flux - 2×10^6 neut/cm^2 sec with 9' collimation λ = 1.015 Å
	Wide-angle time-slicing diffractometer	Beam size - 2 x 3.7 cm max. Flux - 2×10^6 neut/cm^2 sec with 9' collimation λ = 1.015 Å 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 3×10^{14} n/cm^2 sec. The source has some unique characteristics that promise to open up new scientific opportunites:

- 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 momemtum 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-I 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

SNR/PSR SPALLATION NEUTRON SOURCE

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

The SNR/PSR (Spallation Neutron Research/Proton Storage Ring) 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 the SNR using the advantages of time-of-flight methods. The facility supports a national neutron scattering user program. Available instruments in the user program are: a) a general purpose powder diffractometer; b) a single crystal diffractometer based on the Laue-TOF technique; and c) a filter difference spectrometer for chemical and optic mode spectroscopy. A considerable effort is directed toward pulsed source instrument development including, currently, a constant Q spectrometer, a chopper spectrometer, an electron volt spectrometer, and a liquid and amorphous diffractometer. A proton storage ring (PSR) is under construction and by 1985 the SNR/PSR 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

Two thirds of the neutron scattering beam time on user instruments at the SNR/PSR is allocated by a nationally appointed Program Advisory Committee. Application for instrument time can be made by submitting a completed proposal form for consideration by the PAC. The PAC evaluates proposals on the basis of scientific excellence and optimal use of SNR/PSR 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 SNR/PSR 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

SNR/PSR

TECHNICAL DATA

	1984	1985
Proton Source	LAMPF	LAMPF + PSR
Proton Source Current	1000μA	1000μA
Proton Source Energy	800MeV	800MeV
SNR Proton Current	5μA	100μA
Proton Pulse Width	6μs	0.27μs
Repetition Rate	120Hz	12Hz
Epithermal Neutron Current (n/eV.Sr.S)	$1.6X10^{11}/E$	$3.2X10^{12}/E$
Peak Thermal Flux ($n/cm^2.S$)	$5x10^{13}$	$2x10^{16}$

User Instrument

General Purpose Powder Diffractometer	Liquids and amorphous metals, powder diffraction wave vector $0.3\text{-}50A^{-1}$ resolution 0.45% powder 2% liquids
Single Crystal Diffractometer	Laue time-of-flight spectrometer wave vector $1\text{-}15A^{-1}$ resolution 2% typical
Filter Difference Spectrometer	Inelastic neutron scattering, vibrational spectroscopy energy trans. 35-600 MeV resolution 5-7%

NATIONAL CENTER FOR SMALL-ANGLE SCATTERING RESEARCH

Solid State Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

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	(615) 574-5232	FTS: 624-5232
G. D. Wignall, SANS-NCSASR	(615) 574-5237	FTS: 624-5237
J. S. Lin, SAXS-NCSASR	(615) 574-4534	FTS: 624-4534
G. J. Bunick, SANS-NCSASR	(615) 576-2685	FTS: 626-2685
M. Gillespie, Secretary NCSASR	(615) 574-5231	FTS: 624-5231

Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

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 Å or 2.38 Å

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: $5 \times 10^{-3} \leq K \leq 0.6$ Å^{-1}

Detector: 64 by 64 cm^2

Flux at specimen: 10^4–10^6 neutrons/cm^2 sec depending on slit sizes and wavelength

10-m SAXS Instrument Specifications

Monochromator: hot-pressed pyrolytic graphite

Incident wavelengths: 1.542 Å (CuK_α) or 0.707 Å (MoK_α)

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: $3 \times 10^{-3} \leq K \leq 0.3$ Å^{-1} (CuK_α)

$6 \times 10^{-3} \leq K \leq 0.6$ Å^{-1} (MoK_α)

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 μs for oscillatory experiments or 10 s for transient relaxation experiments) and interactive graphics for data analysis

STANFORD SYNCHROTRON RADIATION LABORATORY

Stanford University
Stanford, California 94305

SSRL is a national facility for the utilization of synchrotron radiation. The radiation comes from the 4 GeV storage ring, SPEAR. SPEAR is dedicated to the production of synchrotron radiation half of its operating time. During this time, high currents (up to 100 mA) of electrons are stored at high energy (3-3.5 GeV). The other half of the time, the ring operates for both colliding beam physics and synchrotron radiation under conditions established by the high energy physics program.

Specific research performed at SSRL is extremely varied and includes, in the vacuum ultraviolet area: ionization properties of small molecules, structural and electronic properties of microstructures, properties of ultra-thin layers and small clusters, kinetic process in laser materials, lithography and microscopy, and static properties and dynamic processes of chemisorbed gases. Presently research in the chemical and biological sciences includes: the structure and function of homo- and heterogeneous catalysts, the structure of metal, metal oxide and semiconductor surfaces and their interactions with small molecules, chemical reactivities in the gas phase, the structure of general chemical compounds through EXAFS, multiple wavelength imaging, protein structures and functions through diffraction studies in the crystalline state, protein structures through EXAFS studies, dynamics and fluctuations in biological systems, the nature of membrane structures and membrane protein interactions, the structure and function of metal site in metalloproteins and metalloenzymes.

X-ray physics and materials sciences are represented by research in the following areas: structure of amorphous materials, coordination of impurities and alloying species, structures of and phase transitions in surfaces and thin surface layers, kinetics of structural changes in materials, phase transitions at high pressure, structure of crystalline materials, electronic structure of materials through edge absorption studies, fundamental X-ray scattering and absorption physics, and atomic physics.

Presently SSRL has 18 experimental stations on 6 beam lines covering the spectrum from 6-45,000 eV. 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.

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% of all active proposals receive beam time.

PERSON TO CONTACT FOR INFORMATION

K. M. Cantwell
SSRL, Bin 69 P. O. Box 4349
STANFORD, CA 94305

(415) 854-3300 ext. 3191
(FTS) 461-9300 ext. 3191

CHARACTERISTICS OF SSRL EXPERIMENTAL STATIONS

	Horizontal Angular Acceptance (Mrad)	Energy Range (eV)	Resolution	Approximate Spot Size Hgt x Wdth (mm)	Remarks
Beam Line I					
1-1 (4^{o})	2.0	32-1000	$\Delta\lambda$=.1-.2A	2.0 x 1.0	Double Focus
1-2 (8^{o})	4.0	4-40	$\Delta\lambda$=.2-6A	1.0 x 3.0	Highly Polarized Double Focus
1-4 (Curved Crystal)	2.2	6000-9500	$\sim$ 60 eV	0.25 x 0.5	Double Focus Scattering
1-5 (EXAFS I)	1.0	3800-29300	$\Delta\lambda E/E \sim 10^{-4}$	2.0 x 20.0	Rapidly Tunable
Beam Line II					
II-2	4.8	2800-8900	$\Delta E/E \sim 5x10^{-4}$	2.0 x 4.0	Rapidly Tunable
II-3	1.0	2800-30000	$\Delta E/E \sim 5x10^{-4}$	2.0 x 20.0	Rapidly Tunable
II-4	1.0	3200-30000	White Radiation	4.0 x 15.0	
Beam Line III					
III-1 (4^{o})	2.0	15-1200	$\Delta\lambda$ =.05-2A	1.0 x 1.0	Double Focus
III-3 (2^{o})	8-10	800-4000	0.35-7 eV	2.0 x 4.0	Ultra High Vacuum
III-4 (3^{o})	2.0	2-3000	White or $\Delta\lambda/\lambda$ =.01	2 x 8	Differentially Pumped
Beam Line IV (Wiggler)					
IV-2					
Unfocused	1.0	2800-45000	$\Delta E/E \sim 10^{-4}$	2.0 x 20.0	Rapidly Tunable
Focused	4.6	2800-10200	$\Delta E/E \sim 5x10^{-4}$	2.0 x 6.0	
IV-3 & IV-1	1.0	2800-45000	$\Delta E/E \sim 10^{-4}$	2.0 x 20.0	Rapidly Tunable
Beam Line VI (Wiggler)					
VI-2					
Unfocused	1.0	2800-45000	$\Delta E/E \sim 10^{-4}$	2.0 x 20.0	Rapidly Tunable
Focused	3.0	2800-21000	$\Delta E/E \sim 5x10^{-4}$	2.0 x 6.0	
Beam Line VII (Wiggler)					
VII-1 (Rotation Camera)	1.0	4500-8500	$\Delta E/E \sim 8x10^{-4}$	0.6 x 3.0	Double Focus
VII-2					
Unfocused	1.0	2800-45000	$\Delta E/E \sim 10^{-4}$	2.0 x 20.0	Rapidly Tunable
Focused	4.6	2800-10200	$\Delta E/\sim 5x10^{-4}$	2.0 x 6.0	
VII-3	1.0	2800-45000	$\Delta E/E \sim 10^{-4}$	2.0 x 20.0	Rapidly Tunable
Beam Line 0-0 (Lifetimes Port)	1.8	1-6	Bandpass 10A	4.0 x .4	Pulsed Visible Light

June 18, 1984

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 and a demonstrated lattice resolution of 3.5 Å. This HVEM is interfaced to two accelerators, a National Electrostatics 2MV 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. 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 opposite 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 CX transmission and scanning transmission electron microscope (TEM/STEM), equipped with an x-ray energy dispersive spectrometer (XEDS), and a Philips EM 400 TEM 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, ultra-high vacuum AEM will operate up to 300 keV and have the highest available microanalytical resolution. 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 unique facilities of the Center should submit a proposal to the person 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 TO CONTACT FOR INFORMATION

A. Taylor (312) 972-5109
Electron Microscopy Center for Materials Research FTS 972-5109
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 Magnification 63-1,000,000X Continuous voltage selection (100-1200 kV) Curent 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 K - 1300 K Straining and environmental stages
Transmission Electron Microscope Philips EM 400 (120 keV)	Resolution 2.0 Å lattice Equipped with EELS, XEDS Specimen stages 78 K - 900 K
Transmission Electron Microscope JEOL 100 CX (120 keV)	Resolution 2.0 Å lattice Equipped with STEM, XEDS Specimen stages 78 K - 900 K
Analytical Electron Microscope Being acquired (300 keV)	State-of-the-art resolution Ultra-high vacuum Equipped with EELS, XEDS, etc.
Accelerators	
NEC Model 2 UDHS	Terminal voltage 2 MV Energy stability ± 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 ± 300 eV Current density: He^+, 200 μA/cm^2 (typical) Ni^+, 2 μA/cm^2

SHARED RESEARCH EQUIPMENT PROGRAM (SHaRE)

Metals and Ceramics Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

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, surface analysis, and nuclear microanalysis. The electron microscopy capabilities include high resolution, high voltage in situ studies, and analytical [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; ion backscattering and nuclear reaction techniques using the 0.4 and 5.0 MV Van de Graaff accelerators in the Metals and Ceramics Division.

USER MODE

User interactions are through collaborative research projects between users and researchers on the Materials Sciences Program at ORNL. Proposals are reviewed by an executive committee which consists of ORAU, ORNL, and university members. Current members are Drs. E. A. Kenik, Chairman, P. S. Sklad, J. J. Hren, R. F. Davis, and R. E. Wiesehuegel. Proposals are evaluated on the basis of scientific excellence and relevance to DOE needs and must identify one ORNL staff member who 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 37830
(615) 574-5066
FTS 624-5066

A. Wohlpart
Oak Ridge Associated Universities
P.O. Box 117
Oak Ridge, Tennessee 37830
(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; electron irradiation studies; ten 4-h shifts/week; available evenings, weekends to qualified users
Philips EM400T/ FEG Analytical Electron Microscope	TEM resolution <0.16 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
JEOL 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
JEOL 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 μm 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 MW 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	To be delivered late FY 1984
Atom Probe/ Imaging Atom Probe/Field Ionization Microscope	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 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, microcrystal-lography, 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 rsearch 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 Charactersitcs
Imaging Secondary Ion Microprobe Cameca IMS 3f	Dual ion sources (C_s^+,O_2^+). Depth profiling and mass analyzed secondary ion images with 1μm resolution.
Scanning Auger Microprobe Physical Electronics 595	Resolution: SEM 30 nm, Auger 70 nm. Windowless X-ray detector.
Scanning Auger Micropobe 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)	Delivery June 1984, EDS, EELS.
Transmission Electron Microscope Philips EM420 (120kV)	EDS. Cold stage (30K). Computer Control.
Transmission Electron Microscope Philips EM400T (120kV)	EDS. Heating, cooling stages.
Scanning Transmission Electron Microscope Vacuum Generators HB 5 (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, a spark-source mass spectrometer, optical microscopes, a surface profiler, a microhardness tester, etc. Dark rooms and full specimen preparation facilities are available, including five ion-milling stations, evaporators, 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 37830

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

B. R. Appleton
Solid State Division
Oak Ridge National Laboratory
Post Office Box X
Oak Ridge, Tennessee 37830

(615) 574-6283
FTS 624-6283

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 μamps.
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 μamps doubly and triply charged.
0.1—10-KeV Ion Gun	Gaseous species. ∿20 μamps.
Lasers	
Pulsed Ruby Laser (0.6943 μm)	15—30 x 10^{-9} s pulse duration time. 10 Joule/Pulse Output Multimode, 2 Joule/Pulse Output Single Mode (TEM_{oo}).
Pulsed Ruby Laser (0.6943 μm)	15—30 x 10^{-9} s pulse duration time. 8 Joule/Pulse Output Single Mode (TEM_{oo}).
Pulsed Excimer Laser (0.249 μm)	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 spontaneous Raman spectroscopy, are being developed and used to study high-temperature corrosion and erosion of materials exposed to combustion environments. Emphasis is on the use of these techniques to identify chemical compounds present on surfaces during attack and the resultant effects on structural phase 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 corrosive 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 is the Atmospheric Combustor Exhaust Simulator, which is instrumented for Raman spectroscopy and provides a realistic environment for corrosion and erosion studies relevant to combustion systems. Real-time measurements are complemented by post-exposure techniques such as Raman spectroscopy with sputtering, scanning Auger spectroscopy, low-energy electron diffraction, x-ray diffraction, and metallographic analysis to provide additional compositional and morphological information.

USER MODE

The materials program at the Combustion Research Facility has emphasized research into corrosion and erosion mechanisms using the techniques and apparatus described above. Interactions include: (1) collaborative research projects with outside users, and (2) technology transfer of new diagnostic approaches for the study of material attack. In initiating collaborative research projects, it is desirable to perform preliminary Raman analyses of typical samples and of reference materials to determine the suitability of Raman spectroscopy to the user's particular application. Users interested in exploring potential collaborations should contact the person 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.

PERSON TO CONTACT FOR INFORMATION

Richard E. Palmer
Division 8354
Sandia National Laboratories
Livermore, California 94550

(415) 422-3126
FTS 532-3126

COMBUSTION RESEARCH FACILITY - MATERIALS PROGRAM

TECHNICAL DATA

Instruments	Key Features	Comments
Raman Surface Analysis System	UHV Chamber; Raman system with Ar laser, triple spectrograph and OMA; scanning Auger; sputtering capability.	Simultaneous Raman and sputtering. Raman system capable of detecting 22 nm thick oxides, up 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 OMA.	Cavity-dumped Ar laser and Cu-vapor laser allow gated detection for black-body background rejection. 50 micron x 2 mm spatial resolution. Sample heating up to 1000C. Up to 10 spectra per second.
Atmospheric Combustor Simulator	Raman system with Ar laser, scanning triple	Burns methane or fuel oil. 6 m/s flow. 1000C temperatures. Particulate and impurity gas injection.

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 inquires 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			
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

CENTER FOR X-RAY OPTICS

Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720

The Center for X-Ray Optics was created in August, 1983 to take the lead in developing new optical components and techniques for both science and industry. In the few months of its existence, the Center has begun to develop and use new technologies for the efficient transport, focusing, dispersion, and detection of radiation with photon energies extending from 20 eV to many keV, as well as the production of classical and coherent x-ray sources. Already established programs include microfabrication techniques, mirror technology, pulsed sources, and the development of coherent XUV radiation.

One major goal of the new Center is to provide a national resource for scientists working with radiation in the above spectral regions, including those at the various soft x-ray and VUV synchrotron radiation facilities. Specific plans include developmental work on reflective and diffractive optics, multilayer coatings for extending x-ray interference capabilities, picosecond x-ray detectors, developing a soft x-ray standards laboratory, and participation in undulator and high gain FEL experiments appropriate for this spectral region.

USER MODE

Collaboration with scientists active in this technical area.

PERSON TO CONTACT FOR INFORMATION

David Attwood
Center for X-Ray Optics
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

(415) 486-4463, or
FTS 451-4463

TECHNICAL DATA/FACILITIES

New laboratories and collaborations being organized.

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 1.5 MeV Kratos microscope dedicated largely for in-situ work, a 1 MeV JEOL atomic resolution microscope (ARM), and a high-resolution feeder microscope (JEOL 200CX). 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; W. L. Bell, J. M. Gibson, D. A. Howitt, A. Simnad, J. C. H. Spence, and A. Taylor; 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, CA 94720

(415) 486-6062, or
FTS 451-6062

NATIONAL CENTER FOR ELECTRON MICROSCOPY

TECHNICAL DATA

Instruments	Key Features	Characterization
KRATOS 1.5 MeV Electron Microscope	Resolution 3Å (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 $\leq$ 1.7Å (pt-pt) over full voltage range. Ultrahigh resolution goniometer stage, $\pm 40^\circ$ 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 HVE
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 diameter specimens
200 kV dedicated Analytical Electron Microscope	X-ray and energy-loss spectrometers microdiffraction (CEB)	100 kV - 200 kV LaB_6 filament, state-of-the-art resolution

SECTION E

Summary of Funding Levels

SUMMARY OF
FUNDING LEVELS

During the fiscal year ending September 30, 1984, the Materials Sciences total support level amounted to about $125.1 million in operating funds (budget outlays) and $12.7 million in equipment funds. The following analysis of costs is concerned only with operating funds (including SBIR) i.e., equipment funds which are expended primarily at Laboratories are not shown in the analysis. 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, DL, MA, MD, ME, NJ, NH, NY, PA, RI, VT)	47.3	26.4
(b) South..... (AB, AR, FL, GA, KY, LA, MS, NC, SC, TN, VA, WV)	8.2	18.7
(c) Midwest..... (IA, IL, IN, MI, MN, MO, OH, WI)	23.2	29.7
(d) West..... (AZ, CO, KS, MT, NB, ND, NM, OK, SD, TX, UT, WY, AK, CA, HW, ID, NV, OR, WA)	21.3	25.2
	100.0	100.0

2. By Discipline:

	Contract and Grant Research (% by $)	Total Program (% by $)
(a) Metallurgy, Materials Science, Ceramics (Budget Activity Numbers 01-)	60.0	39.0
(b) Physics, Solid State Science, Solid State Physics (Budget Activity Numbers 02-)	33.0	50.3

SUMMARY OF
FUNDING LEVELS

	Contract and Grant Research (% by $)	Total Program (% by $)
(c) Chemistry, Chemical Eng. (Budget Activity Numbers 03-)	6.7	10.7
	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)...	36.8
(b) DOE Laboratory Programs.....	62.0
(c) Industry and Other.....	1.2
	100.0

4. By Laboratory and Contract and Grant Research

	Total Program (%)
Ames Laboratory	6.0
Argonne National Laboratory	16.8
Brookhaven National Laboratory	18.3
Idaho National Engineering Laboratory	0.4
Illinois, University of (Materials Research Laboratory)	2.6
Lawrence Berkeley Laboratory	10.6
Lawrence Livermore National Laboratory	1.2
Los Alamos National Laboratory	3.1
Oak Ridge National Laboratory	16.8
Pacific Northwest Laboratory	1.6
Sandia National Laboratories	3.3
Solar Energy Research Institute	0.3
Stanford Synchrotron Radiation Laboratory	0.6
Contract and Grant Research	18.4
	100.0

23018
3253
26271

SUMMARY OF
FUNDING LEVELS

37.5

5. By Selected Areas of Research:

	% of Prorated Projects[a] (Total=415)	% of Program Funding[a] ($125.1 million)	% of Individual Projects[c] (Total=415)
Materials			
Ceramics (Crystalline)	18.0	15.0	25.0
Ferrous Alloys	6.2	3.9	17.3
Intermetallics	3.9	3.3	9.4
Polymers	4.1	2.4	6.2
Semiconductors	8.2	7.2	13.0
Technique			
Electron Microscopy (Technique Development)	3.2	2.8	7.2
Neutron Scattering	4.7	17.8	9.2
Synchrotron Radiation	3.0	10.3	5.1
Theory	14.0	11.2	37.6
Phenomena			
Catalysis	2.7	2.8	6.7
Corrosion	6.1	4.5	10.4
Diffusion	5.8	4.2	14.2
Processing Science/Synthesis[b]	16.1	12.3	29.6
Strength	9.3	4.8	16.1
Superconductivity	3.8	3.7	6.3
Environment			
High Temperature (> 1200°K)	4.4	4.0	6.3
Radiation	5.1	11.4	9.0
Sulfur-Containing Gases	1.5	1.3	2.9

[a]The funding levels and projects percentage for various research categories were determined from the index listing in Section F and estimating the percentage from the project devoted to a particular subject. There is overlap in the figures. For instance, funding for a project addressing creep of oxides would appear in the categories of ceramics, strength, and (possibly) high temperature.

[b]Based on projects indexed in Section F 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 F

Index of Investigators, Materials, Techniques, Phenomena and Environment

The following indexes refer to project numbers in Sections A, B and C.

INVESTIGATORS

INVESTIGATORS

INVESTIGATORS

INVESTIGATORS

INVESTIGATORS

INVESTIGATORS

INVESTIGATORS

INVESTIGATORS

INVESTIGATORS

TECHNIQUES

X-Ray Scattering and Diffraction (wide angle crystallography)

002, 019, 023, 024, 026, 027, 028, 048, 073, 079, 081, 085, 106, 113
118, 130, 132, 152, 154, 205, 216, 238, 245, 261, 263, 267, 303, 315
319, 324, 330, 348, 361, 362, 371, 377, 383, 390, 393, 394, 397, 402
403, 404, 418, 424, 436, 450, 479, 480, 486, 491

X-Ray Scattering (small angle)

079, 085, 106, 118, 154, 176, 221, 236, 245, 276, 311, 394, 403

X-Ray Scattering (other than crystallography)

019, 047, 085, 106, 176, 216, 340, 362, 394, 445, 447, 490

X-Ray Photoelectron Spectroscopy

008, 018, 024, 025, 052, 074, 085, 106, 176, 203, 241, 262, 264, 278
295, 351, 394, 411, 426, 439, 471, 474, 478

PHENOMENA

ENVIRONMENT

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