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Materials Sciences Programs
Fiscal Year 1983

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, Mathematical 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, and Chemistry. The structure of the Division is given in an accompanying chart.

The Materials Sciences Division conducts 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 1983 together with a convenient index to the program. Recent publications from Division-sponsored panel meetings and workshops are listed on the next page.

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[b]

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

- Ceramic Processing
- Erosion and Wear
- High Voltage Electron Microscopy
- Non-Destructive Evaluation
- Sulfur Attack
- Welding

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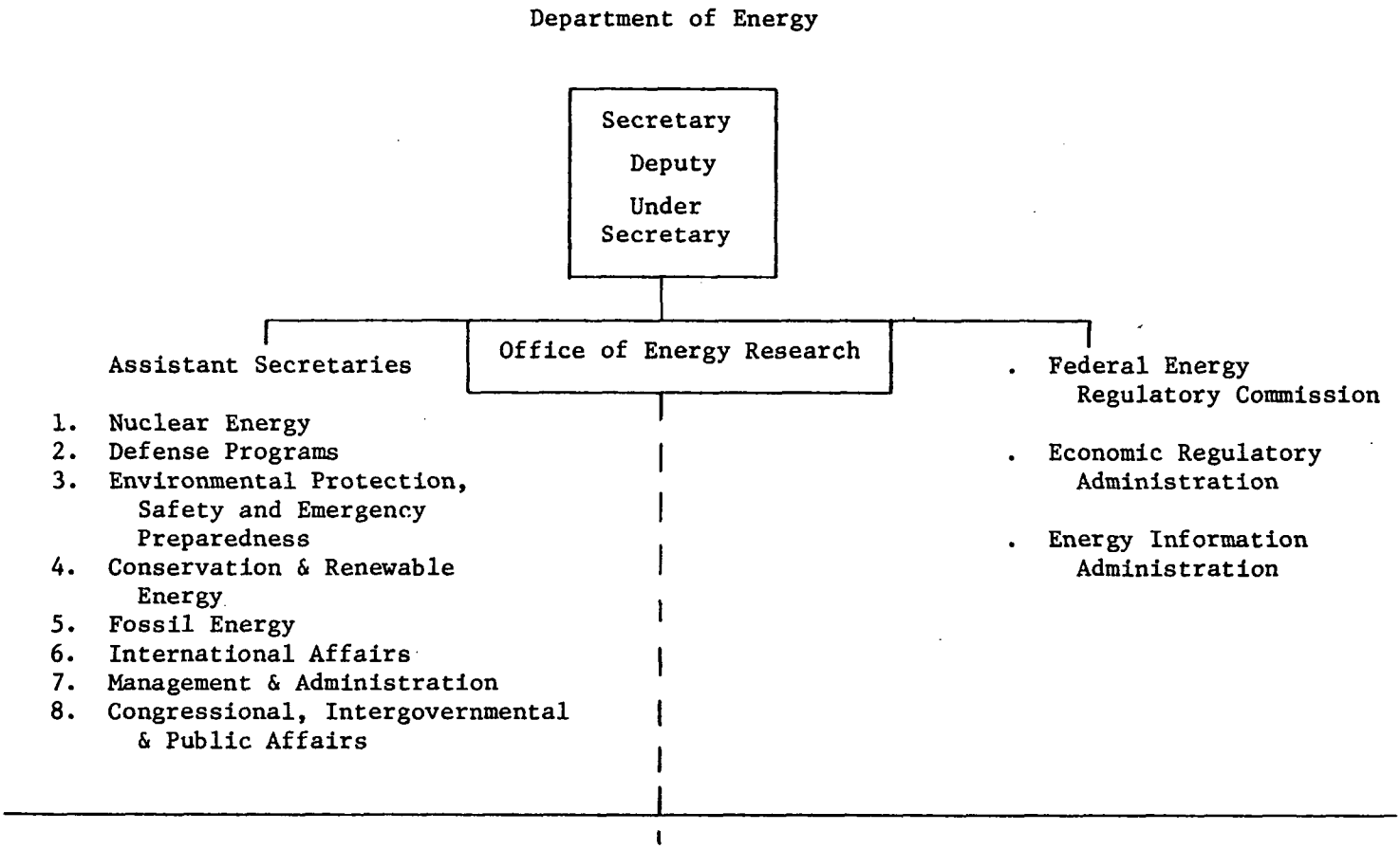
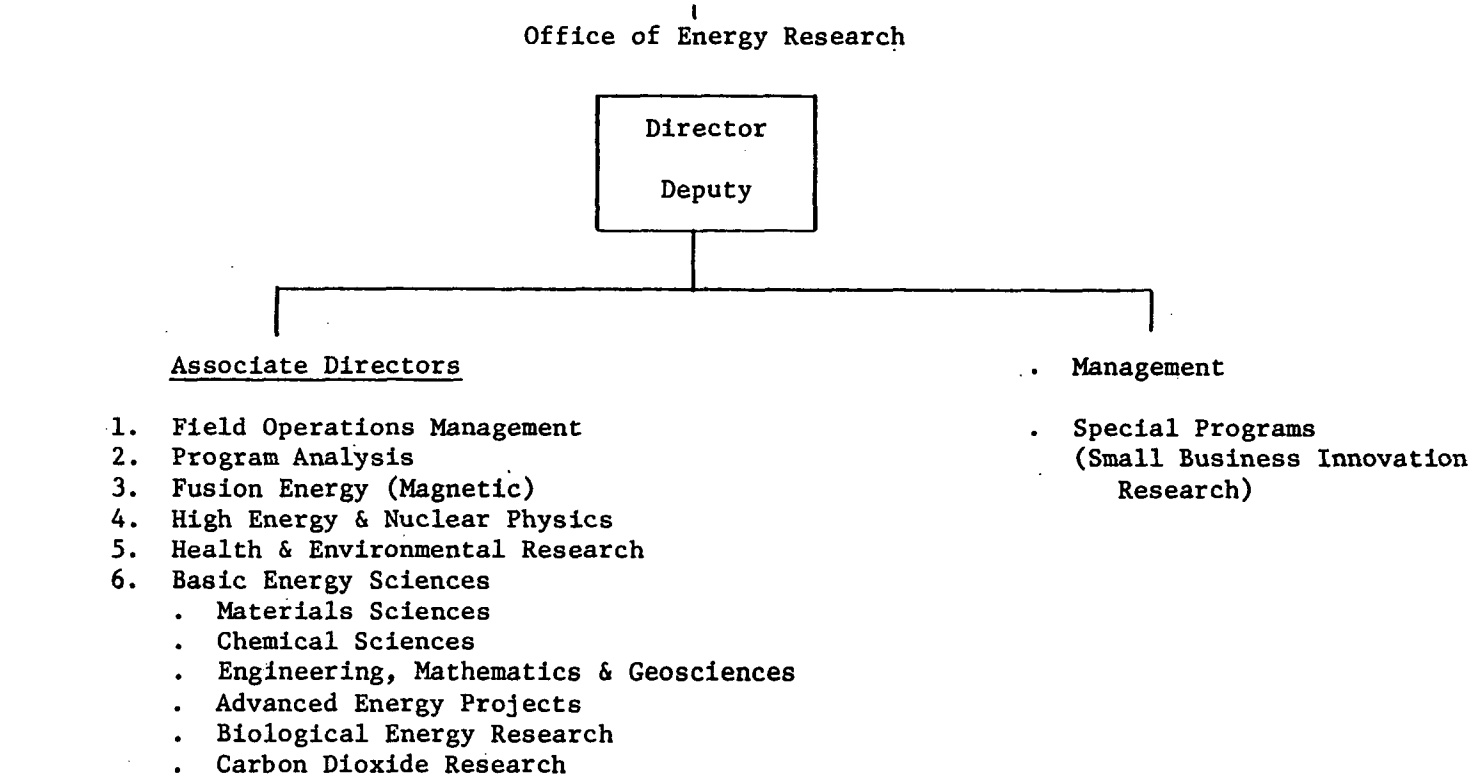
[a] Available in limited quantities from the Division of Materials Sciences.
[b] To be published.
[c] Also published in Materials Science and Engineering.

ORGANIZATION OF THE DEPARTMENT OF ENERGY

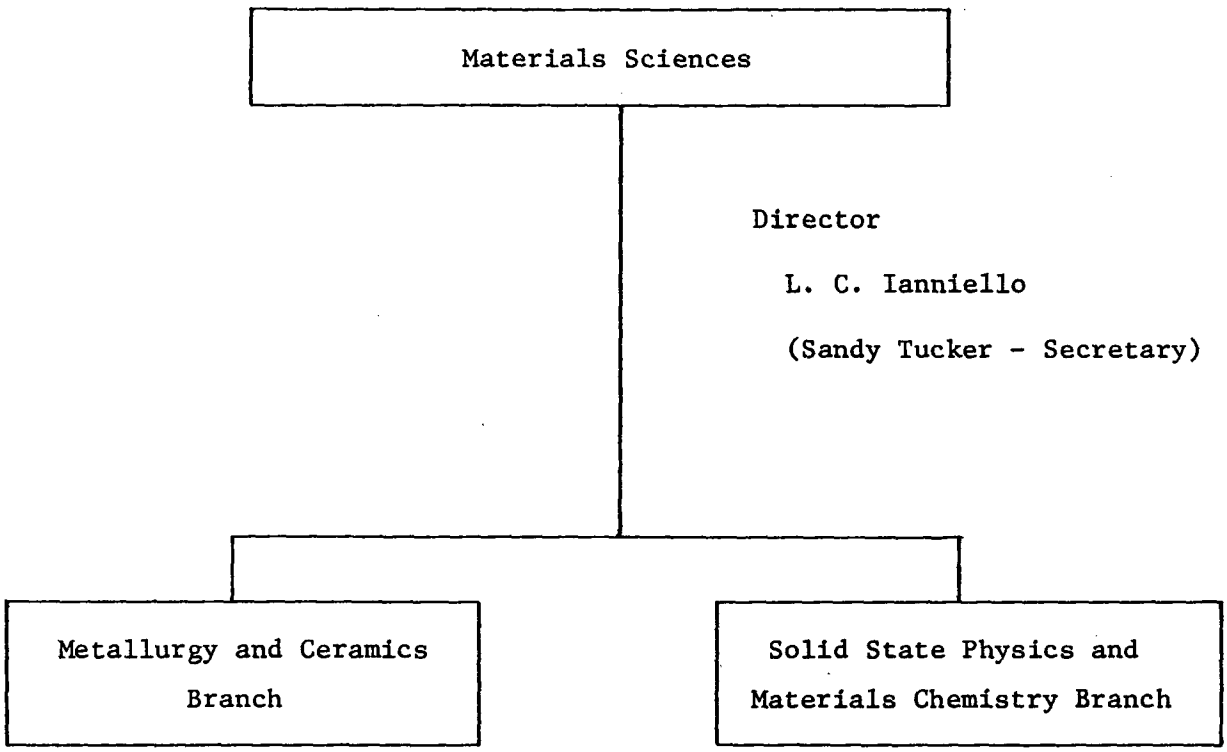




STRUCTURE OF

DIVISION OF MATERIALS SCIENCES

OFFICE OF BASIC ENERGY SCIENCES



(Janet Venneri - Secretary)

Chief: Vacant
S. M. Wolf
R. J. Gottschall
F. V. Nolfi, Jr. 1/
D. M. Parkin 2/

(Linda Twenty - Secretary)

Chief: M. C. Wittels
T. A. Kitchens
B. C. Frazer 3/
J. B. Darby, Jr. 4/
M. Weber 5/
H. G. Smith 6/

Notes:
1/ On Leave from Ames Laboratory
2/ Return to Los Alamos National Laboratory 7/83
3/ On Leave from Brookhaven National Laboratory
4/ Return to Argonne National Laboratory 10/83
5/ On Leave from Lawrence Livermore National Laboratory
6/ 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 intended for use by administrators, managers, and scientists to help coordinate research and as an aid in selecting new programs.

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 shows distribution 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 1983 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. All 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 such a large program. By the time it could be compiled it would be outdated. The best method for obtaining more detailed information about a given research project is to contact directly the investigators listed.

Preparation of this FY 1983 summary report was coordinated by S. M. Wolf.

TABLE OF CONTENTS

SECTION A - Laboratories

SECTION B - 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 on pages 1 through 74 was provided by the Laboratories. Most projects are of a continuing nature although specific projects were concluded and others initiated in FY 1983.

LABORATORIES

AMES LABORATORY
Iowa State University
Ames, Iowa 50011
R. S. Hansen - Phone (FTS) 865-2770 or 515-294-2770

Metallurgy and Ceramics - 01-
F. V. Nolfi - Phone (FTS) 865-4446 or 515-295-4446

1. SURFACES AND SOLIDIFICATION
R. K. Trivedi, J. T. Mason, A. Roy
Phone: (515)-294-5869

$180,000 01-1

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

2. MICROSTRUCTURAL CONTROL IN METALS
J. D. Verhoeven, E. D. Gibson
Phone: (515)-294-9471

$285,000 01-1

Production of Nb_3Sn-Cu and V_3Ga-Cu superconducting wire by the in situ process: development of a roll bonding technique to evaluate flux pinning mechanisms and problems in the addition of Sn by the external diffusion method, evaluation of Nb_3Sn filament cross linking within the microstructure, and determination of the effect of residual Si levels on V_3Ga-Cu wire produced by both the in situ and conventional bronze routes. A study of directionally transformed pearlite versus applied stress level and temperature gradient. The mechanical properties of in situ prepared Cu-Ta alloys. Directional solidification studies on segregation in grey and nodular cast iron. Evaluation of microstructural changes in the austempering of nodular cast irons.

3. MATERIALS SCIENCE OF INTERFACES
A. J. Bevolo, F. C. Laabs, L. M. Seaverson
Phone: (515)-294-5414

$ 70,000 01-1

Studies of interfaces using Auger, ELS, and SIMS surface analytical techniques in combination with ion etching. Core level and plasmon spectra of pure and oxidized rare earth metals using ELS and Auger. Effects of tin doping of brass on its corrosion behavior in aqueous salt solutions. Scanning Auger microprobe analysis (350Å) 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. Oxidation of liquid and solid tin by ELS. Local chemical state information from Auger lineshape analysis in Fe-B-Be metallic glasses and Mg_2X (X=Si, Ge, Sn, Pb).

AMES LABORATORY (continued)

4. NONEQUILIBRIUM MATERIALS
J. D. Verhoeven, R. K. Trivedi, A. J. Drehman, A. R. Pelton
Phone: (515)-294-9471

$ 70,000 01-1

This is a new area of research which will focus on metallic glasses, metastable crystalline phases and extremely fine microstructural alloys. For initial experiments a high vacuum melt spinning apparatus is being constructed and a directional solidification apparatus modified to achieve very high solidification rates. High speed planar solidification of eutectic Pb-Cd is being studied as well as the microstructure of rapidly crystallized Si-Ge alloys. Future work will include the investigation of a wide range of metallic alloys.

5. MECHANICAL METALLURGY AND MATERIALS RELIABILITY
O. Buck, J. Kameda, J. Kasichainula, C. V. Owen, D. K. Rehbein, B. J. Skillings
Phone: (515)-294-3930

$540,000 01-2

Effects of hydrogen on crack initiation in refractory alloys under uniaxial and cyclic loading conditions. Internal friction due to hydrogen in solid solution (in collaboration with the Max-Plank Institute, Stuttgart/Germany) and due to hydrides. 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. Microscopic characterization and modeling of the synergetics of stress and deformation on crack initiation under stress corrosion conditions. Ultrasonic characterization of fatigue cracks in alloys exposed to harsh environments. Development of new nondestructive evaluation techniques to determine materials degradation.

6. RARE EARTHS IN STEELS
M. S. Wechsler
Phone: (515)-294-5082

$ 40,000 01-2

Elevated temperature mechanical properties (uniaxial tensile and indentation hardness tests) on ferritic and austenitic steels as a function of rare earth element additions, particularly Y, Ce, and La in concentrations below one percent. Also, irradiation swelling behavior, electron microscopy, and metallography. Application to LMFBR cladding and fusion reactor first wall.

7. SHAPE MEMORY PHENOMENA
M. S. Wechsler
Phone: (515)-294-5082

$ 65,000 01-2

Tensile properties, internal friction, strain and volume change measurements, and resistivity measurements in Ni-Ti as a function of prior transformation fatigue cycling and applied stress.

AMES LABORATORY (continued)

8. THERMODYNAMICS AND PHASE EQUILIBRIA
J. F. Smith
Phone: (515)-294-5083

$ 50,000 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, glass formation, and control of microstructures.

9. ULTRASONIC MEASUREMENTS
J. F. Smith, R. B. Thompson
Phone: (515)-294-5083 - (515)-294-8252

$ 65,000 01-3

Martensitic transformations in ZrO_2 and HfO_2 are responsible for the sensitivity of these materials to thermal shock. Ultrasonic wave velocities are being measured in yttria stabilized single crystals of ZrO_2 at elevated temperatures to determine the role of the elastic constants in the transformations. Acoustoelastic techniques to determine residual stresses in materials with preferred grain orientations with emphasis on the influence of grain and dislocation structures.

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

$200,000 01-3

Study of diffusion and electrotransport of fast diffusing solutes in scandium. Measurement of transport parameters for iron, cobalt and nickel as a function of temperature and determination of activation energy for diffusion. Fast diffusion of cobalt in thorium. Characterization of responsible defect by internal friction studies. Thermotransport of interstitial solutes in one-phase alloys of V and Nb. Mass transport of carbon in two-phase Nb-C and V-C alloys in presence of temperature gradient. Investigation of effect of alloying or impurity elements on ductility transition temperature of Fe-9Cr-1Mo steel using slow, notch-bend and Charpy impact tests. Effect of 500°C aging on ductility of tempered alloys for high purity base alloys and Oak Ridge modified ferritic steel.

11. HYDROGEN IN METALS
D. T. Peterson
Phone: (515)-294-6585

$250,000 01-3

Diffusion, thermotransport, and solubility of H and D in V alloys with Ti, Cr, Nb or O. Photoelectron spectroscopy, and metallography of metal hydrides and solid solutions of H in vanadium base alloys.

AMES LABORATORY (continued)

12. TRANSFORMATION STUDIES AND ORDERED ALLOYS
F. X. Kayser
Phone: (515)-294-5874

$ 80,000 01-3

Resistivity measurements of Fe-Si alloys containing 12 to 26 at.% silicon, from 4.2 to 300 K. Fine-scale structural changes, low temperature phase diagram.

13. RARE EARTH MATERIALS
K. A. Gschneidner, Jr., S. K. Dhar
Phone: (515)-294-2272

$185,000 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 $CeSn_x$ ($x \simeq 3$) and $CeSi_x$ ($x \simeq 1.8$) 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. Influence of electron concentration and size on the lattice instability and superconducting properties of rare earth based superconductors: $La_{3-x}S_4$, $La_{3-x}Se_4$ and $(La_{1-x}Th_x)_{3-y}S_4$.

14. NDE MEASUREMENT TECHNIQUES
R. B. Thompson
Phone: (515)-294-8252

$155,000 01-5

Techniques to measure failure related material properties are investigated. Dual objectives of improving understanding of failure mechanisms and inspection reliability. 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.

15. PROPERTIES AND PROCESSING OF CERAMICS
M. F. Berard, M. Akinc, G. W. Jordan, M. D. Rasmussen
Phone: (515)-294-6964

$290,000 01-5

Phase equilibria and electrical conductivity studies in binary and ternary oxides based on HfO_2 and ZrO_2. 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.

AMES LABORATORY (continued)

16. MATERIALS PREPARATION AND PROCESSING (also see page 180)
F. A. Schmidt, O. D. McMasters
Phone: (515)-294-5236 - (515)-294-3630

$275,000 01-5

Processing of refractory and strategic metals. New process for preparing kilogram quantities of high purity vanadium. New techniques for processing thorium from ThF_4 and for the metallurgical upgrading of cobalt metal. Development of arc melting procedures for preparing Cu-Nb, Cu-Ta and Cu-Mo alloys containing uniform dispersion of the refractory metal. Effect of silicon on the critical current density J_c in V_3Ga. 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. Single crystals (1-2 cm^3) of pure metals, solid solution alloys, intermetallic compounds, both congruent melting and peritectic in nature. Directionally solidified materials for specific applications. Methods available-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.

Solid State Physics Division - 02-
D. K. Finnemore - Phone (FTS) 865-3455 or 515-294-3455

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

$350,000 02-1

Study of the lattice dynamics, thermodynamic properties and structural transformations of metals at high temperatures (Mo, 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).

18. SEMICONDUCTOR PHYSICS
H. R. Shanks
Phone: (515)-294-6816

$220,000 02-2

Preparation and characterization of thin films, rf sputter desposition of amorphous semiconductors including a-Si, a-SiC, a-Ge, a-GeC and AlN, electron beam deposition of Si, heteroepitaxy on compound substrates, surface and interface characterization with LEED, Auger, LEELS, photodeflection and ir absorption spectroscopy for bonding studies, measurements of gap state densities using DLTS and C-V on Schottky barriers.

AMES LABORATORY (continued)

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

$390,000 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; supercurrents in normal metals near a superconductor normal metal boundary; quantum interference phenomena 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.

20. OPTICAL AND SPECTROSCOPIC PROPERTIES OF SOLIDS AND LIQUIDS
D. W. Lynch, C. G. Olson, D. M. Wieliczka
Phone: (515)-294-3476

608-873-6651
608-262-8946

$350,000 02-2

Electron photoemission and optical properties (transmission, reflection, EXAFS, thermoreflection, thermotransmission, of solids in the near infrared, visible, vacuum ultraviolet and soft X-ray region using synchrotron radiation): transition metal alloys and compounds (e.g., NiAl, Fe_3Al), layered transition metal chalcogenides ($MoSe_2$), Ce; electroreflectance of Ag in electrolytes. Raman Scattering.

21. NEW MATERIALS AND PHASES
R. N. Shelton, C. A. Swenson, R. G. Barnes, M. S. Anderson, P. Klavins, D. R. Torgeson, J. S. Schilling
Phone: (515)-294-5435

$440,000 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 of interstitial impurities in these metals, structural and electronic characterization of hydrogenated amorphous silicon films.

AMES LABORATORY (continued)

22. MATERIALS FOR HYDROGEN STORAGE
R. G. Barnes, J. D. Corbett, K. A. Gschneidner, Jr., W. A. Kamitakahara, D. T. Peterson, R. J. Schoenberger
Phone: (515)-294-4754

$180,000 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.

23. X-RAY DIFFRACTION PHYSICS
J.-L. Staudenmann
Phone: (515)-294-3585

$200,000 02-2

X-ray diffraction studies of martensitic phase transitions (V_3Si and Fe-C) and electron charge densities; small angle scattering, EXAFS, microdiffraction. Studies of electron density near interstitial impurities. MATRIX PRT beam line at NSLS.

24. ELECTRONIC AND MAGNETIC PROPERTIES
B. N. Harmon, K.-M. Ho, M. Luban, D. Misemer, M. Nolan
Phone: (515)-2984-7712

$400,000 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.

25. OPTICAL AND SURFACE PHYSICS THEORY
R. Fuchs, K. M. Ho, S. Auluck
Phone: (515)-294-3675

$150,000 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. Photoemission and electroreflectance with emphasis on surface states. Photoemission into liquid electrolytes and related catalytic, electrochemical, adsorption, and corrosion effects; anodic photocurrents; the liquid-metal interface.

AMES LABORATORY (continued)

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

$110,000 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; flux-flow voltage noise; vortex nucleation and surface pinning; flux-line cutting in arrays of nonparallel vortices; critical currents and flux pinning in inhomogeneous superconductors; instabilities; ac losses; superconducting magnetic shielding.

Materials Chemistry Division - 03-
L. E. Burkhart - Phone (FTS) 865-8074 or 515-294-8074

27. X-RAY AND NEUTRON CRYSTALLOGRAPHY
R. A. Jacobson, B. J. Helland
Phone: (515)-294-8444

$185,000 03-1

Development of diffraction techniques for single crystal and non-single crystal specimens; indirect methods and refinement techniques; operation of X-ray characterization facility; radial distribution function analysis of amorphous scattering from coal; structural studies of intramolecular solid state interactions which modify properties of parent species; metal complex structures with emphasis on model homogeneous catalysts and polymetal species; coordination numbers and oxidation states for complex molybdates and sulfides using EXAFS.

28. METAL-METAL BONDING IN NEW SOLID STATE MATERIALS
J. D. Corbett
Phone: (515)-294-3086

$170,000 03-1

Materials preparation and characterization of new types of reduced inorganic compounds stable at high temperature (e.g., of Sc, Y, Ti, Zr, Nb, rare earth elements); extended metal-metal bonding; hydrogen storage potential of new types of reduced compounds; chemistry of stress-corrosion-cracking by zirconium; homopolyatomic ions; charge transfer and bonding in Zintl-type phases; crystal structures; photoelectron spectroscopy; electronic structure.

29. STRUCTURE-PROPERTY RELATIONS IN HEAVY TRANSITION METAL PHASES
R. E. McCarley
Phone: (515)-294-8680

$165,000 03-1

Chemistry of heavy transition elements, especially Nb, Ta, Mo, and W. Compounds with strong metal-metal bonding in discrete cluster units and phases with extended metal-metal bonded chains. Ternary and quaternary oxides of molybdenum with metal-clusters and chains. Chemistry of new sulfide compounds with relation to hydrodesulfurization catalysis. Studies of structure and bonding in new oxide and sulfide compounds, and their relationship to physical properties such as electrical and ionic conductivity, mechanical strength, and catalytic activity.

AMES LABORATORY (continued)

30. RECOVERY OF METALS FROM FLY ASH AND OTHER WASTE MATERIALS
G. Burnet, M. J. Murtha
Phone: (515)-294-5840

$170,000 03-2

Recovery from power plant fly ash of iron oxide by magnetic separation and of alumina using calcination; use of magnetic fraction for heavy media in coal preparation plants and source of iron ore; utilization of wastes from fly ash processing plants; X-ray studies of complex metal phosphates found in Portland cement-type wastes from fly ash processing plants; recovery of metals from other fuel processing wastes.

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

$290,000 03-2

Methods for the preparation of ceramic powders; reaction kinetics and control of nucleation, growth rate, and particle size distribution in both liquid phase and vapor phase operations for preparing particulate materials; quantitative description of particle morphology; techniques for modifying particle morphology; quantitative measurement of strength of particle agglomerates; X-ray studies of particulate materials.

32. HIGH TEMPERATURE CHEMISTRY OF REFRACTORY MATERIALS
H. F. Franzen, Bernd Harbrecht
Phone: (515)-294-5773

$245,000 03-3

Fracture and bonding in refractory and corrosion-resistant compounds, particularly metal-rich transition metal chalcogenides (Sc-S and Ta-S), phosphides and aluminides (Zr-Al); stability, phase equilibria, order-disorder transitions, X-ray diffraction, photoelectron spectroscopy, and mass spectrometry studies at high temperatures; band structure and electronic properties of transition-metal sulfides.

33. SURFACE CHEMISTRY AND CATALYSIS
R. S. Hansen, K. G. Baikerikar, D. C. Johnson
Phone: (515)-294-2770

$315,000 03-3

Heterogeneous catalysis, reactions at clean surfaces (including alloy surfaces) associated with coal liquefaction and gasification (e.g., methanation reaction on ruthenium and hydrodesulfurization using non-stoichiometric rare earth sulfides); field emission, flash desorption, LEED and Auger spectroscopy techniques for studying reaction kinetics and composition of surface phases resulting from the interaction of gases such as CO and H_2 on catalyst single crystal faces; electrical double layer properties and their alteration by adsorption, electrochemistry associated with stress corrosion cracking, electrocatalysis at binary electrode surfaces for control of toxic or mutagenic organic molecules (nitrosoamines, polynuclear compounds) in wastes; preparation and electrochemistry of layered chalcogenide photochemical converters (e.g., MoS_2, $MoSe_2$, WSe_2).

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

Materials Science & Technology Division - 01 -

B. R. T. Frost - Phone (FTS) 972-4928 or 312-972-4928
F. Y. Fradin - Phone (FTS) 972-4925 or 312-972-4925
H. Wiedersich - Phone (FTS) 972-5079 or 312-972-5079
F. A. Cafasso - Phone (FTS) 972-4542 or 312-972-4542

34. LAYERED AND THIN FILM MATERIALS
M.B. Brodsky, S.D. Bader, M.H. Grimsditch, R.C. Haushalter, I.K. Schuller, C.S.L. Chun, H.C. Hamaker, G.W. Zajac, G.-G. Zhen
Phone: (312)-972-5016

$ 981,000 01-1

Studies of novel materials properties obtained by thin film techniques--epitaxial sandwiches, multilayered coherent samples and metallic overlayers; room temperature preparation of metallic materials, often metastable and glassy, via Zintl ions. Preparation techniques include atomic (molecular) beam epitaxy and sputter deposition. Materials characterization methods involve magnetic and superconducting properties at low temperatures; atomic structure by TEM and X-ray and electron diffraction; electronic structure changes via AES, UPS, XPS, chemical bonding and theoretical calculations; and vibrational and magnetic excitations by Raman and Brillouin light scattering, neutron scattering and ELS; interface phenomena.

35. 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, B. Chakraborty, G.D. Loper
Phone: (312)-972-4963

$1,223,000 (Does not include H in metals effort) 01-3

Research on the nature and physical properties of intrinsic and extrinsic atomic defects and their interactions in metals, 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; and hydrogen interactions with metallic systems; studies of metals (including refractory bcc metals), alloys, intermetallic compounds, and amorphous metallic systems with experimental techniques such as positron annihilation spectroscopy, radiotracer diffusion, resistometry, 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.

ARGONNE NATIONAL LABORATORY (continued)

36. DEFECTS IN CERAMICS
N.L. Peterson, K. Hoshino, K.L. Merkle, G.E. Murch, J.L. Routbort, J. Sasaki, M. P. Thomas, D. Wolf
Phone: (312)-972-4955
$825,000 01-3

Diffusion mechanisms and point-defect studies in metal oxides as a function of oxygen-partial pressure at high temperatures using 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 nonstoichiometric 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, and alkali-silicon-sulfur glasses; effect of nonstoichiometry and defect clusters on mechanical deformation of oxides; preparation of single and bicrystals of metal oxides.

37. NEUTRON IRRADIATION STUDIES
M.A. Kirk, R.C. Birtcher, S. Egusa, and B.A. Loomis
Phone: (312)-972-4998
$526,000 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; the 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 irradiations; 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 300K.

ARGONNE NATIONAL LABORATORY (continued)

38. KINETICS AND ION IRRADIATION
L.E. Rehn, C.W. Allen, R.S. Averback, J. Don, R.C. Frank, U.F. Kocks, S. Majumdar, P.R. Okamoto, R.B. Schwarz, N.J. Zaluzec
Phone: (312)-972-5021
$1,023,000 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; solute 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; analytical electron microscopy; mechanistic studies of deformation and mechanical strengthening in alloys; theoretical and experimental investigations of solute hardening and dynamic strain aging; radiation sources include HVEM-2MV Tandem facility and two 300 kV ion accelerators.

39. HIGH VOLTAGE ELECTRON MICROSCOPE TANDEM FACILITY (also see page 170)
A. Taylor
Phone: (312)-972-5109
$625,000 01-4

Operation and development of 1.2 MeV High Voltage Electron Microscope Facility with in-situ capability for ion implantation, ion damage, and ion beam analysis; the HVEM is currently being utilized for research programs in mechanical properties, radiation damage, oxidation and hydrogenation effects; specimen stages for heating (1000°C), cooling (9°K), straining, gaseous environments and for the ion-beam interface with a 300 kV ion accelerator and a 2 MV tandem accelerator are available for in-situ implantations and irradiations; approximately 50% of the HVEM usage is by non-ANL scientists on research proposals approved by a steering committee for the HVEM that meets every six months.

ARGONNE NATIONAL LABORATORY (continued)

40. OXIDATION STUDIES
N.L. Peterson. D.J. Baxter, K. Hoshino, W.E. King, K. Natesan, S.J. Rothman, J. Sasaki
Phone: (312)-972-4955
$623,000 01-5

Point defects and diffusion mechanisms in protection-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.

41. NEUTRON AND X-RAY SCATTERING
D.L. Price, T.O. Brun, J.E. Epperson, J. Faber, Jr., G.P. Felcher, J.D. Jorgensen, P.R. Roach, S.K. Sinha, M.H. Mueller, M. Loewenhaupt, B.K. Sarma, C.K. Saw
Phone: (312)-972-5475
$1,397,000 02-1

Use 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; hydrogen in metals, magnetism of intermetallic compounds, alloy decomposition, silicate and chalcogenide glasses, residual stresses in deformed materials, surface magnetism, ternary superconductors, atomic momentum distributions in quantum systems, and nuclear magnetism at ultralow temperatures.

42. CHEMICAL AND ELECTRONIC STRUCTURE
J.M. Williams, C.D. Carlson, R.J. Thorn, A.J. Schultz, M. Beno, P. Leung, H. Horiuchi
Phone: (312)-972-3464
$853,000 02-1

Synthesis and characterization of new materials, especially synthetic organic metals possessing novel electrical properties, dielectric materials, fast oxygen-ion conductors, and compounds that behave as catalysts or model catalysts. Continuing development of the neutron time-of-flight single-crystal diffractometer (SCD), and the U.S. university-industrial users group at the Intense Pulsed Neutron Source. Structure-property relationships for synthetic metals based on TMTSF (tetramethyltetraselenafulvalene) and for organometallic complexes and hydrides which may be active or model catalysts. Variable temperature diffuse scattering and crystal structure studies at the SCD. Development of a very low-temperature (10K) single crystal X-ray facility for electron density and structural studies which require neutron and X-ray data collected at identical temperatures.

ARGONNE NATIONAL LABORATORY (continued)

43. SUPERCONDUCTIVITY AND MAGNETISM
B.D. Dunlap, F. Behroozi, G.W. Crabtree, A.J. Fedro, F.Y. Fradin, K.E. Gray, D.G. Hinks, W.P. Joss, H.C. Li, G.K. Shenoy, A. M. Umarji
Phone: (312)-972-5538

$962,000 02-2

Experimental and theoretical investigations of the magnetic and superconducting properties of materials. Experimental techniques utilized include de Haas-van Alphen effects, Mössbauer spectroscopy, nuclear magnetic resonance, transport measurements, magnetization and susceptibility, electron tunneling, EXAFS and XANES, materials preparation and characterization, and collaborative efforts using neutron scattering, Current topics of interest include: investigations of the relationships between superconductivity and magnetism in the RRh_4B_4 system (R = rare-earth); the role of oxygen impurities in establishing superconducting properties of Chevrel phase systems; superconductivity and magnetism in Heusler phase alloys; Fermi surface studies of narrow band systems, including mixed valence and Kondo lattice phenomena; theoretical investigation of the effect of superconductivity on magnetic exchange coupling; investigation of the electronic properties of organic superconductors; structural studies of chalcogenide gases; design and construction of a soft x-ray beam line at NSLS.

44. MATERIALS PREPARATION AND CHARACTERIZATION AND FAST ION TRANSPORT IN SOLIDS
S. Susman, T. O. Brun, C.J. Delbecq, J.A. McMillan, T. Tokuhiro
Phone: (312)-972-5470

$419,000 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 phosphates and oxides and cyanides. Basic studies are conducted in the microscopics of charge and mass transport in solid electrode and electrolyte materials utilizing neutron diffraction, nuclear magnetic resonance, ionic conductivity, EXAFS and optical spectroscopy. Fast ion transport is examined in mixed electronic and ionic conductors, in skeleton framework compounds and in fast-ion glasses. These include ternary sulphide glasses, Li-Al alloys, NASICON analogs, NASIGLAS, and both crystalline and vitreous β-eucryptites.

ARGONNE NATIONAL LABORATORY (continued)

45. ELECTRONIC STRUCTURE AND BONDING
D.J. Lam, A. T. Aldred, A. J. Arko, S.-K. Chan, G.S. Knapp, J. McMillan, M.V. Nevitt, B.W. Veal, Q.Q. Zheng
Phone: (312)-972-4966
$1,309,000 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; application of differential thermal analysis and Raman spectroscopy to study the devitrification of silicate glasses containing actinides; crystal chemistry and structural stability of complex metal oxides; 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 inelastic neutron scattering measurements; theoretical studies of electron spectra and bonding of ABO_4 and AB_2O_4 compounds; development of molecular cluster code to calculate total energy of embedded AB_2O_4 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.

46. THEORETICAL RESEARCH - CONDENSED MATTER THEORY
D.Y. Smith, L. Guttman, R. Kalia, D. Koelling, A. Rahman, P. Vashishta
Phone: (312)-972-5481
$731,000 02-3

A broad activity in condensed matter theory focusing on statistical physics, electronic structure, and the defect solid state. Current areas of study include: molecular dynamics calculations to model structural phase transitions, melting and nucleation, and fast ion transport in solids; electronic structure calculations of narrow-band materials, including actinides and mixed valence systems; many-body effects in semiconductors, 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.

ARGONNE NATIONAL LABORATORY (continued)

47. GEOPHYSICAL PROSPECTING WITH SQUIDS
R.T. Kampwirth, I.K. Schuller
Phone: (312)-972-5521
$178,000 02-5

The goal of this program is to develop and evaluate instrumentation and data analysis techniques for the location of subsurface hydrocarbon deposits using Superconducting quantum interference Devices (SQUIDS) in conjunction with remote reference Controlled Source Sounding techniques. These results will be compared with Magnetotelluric measurements and well log data where available. Preliminary instrumentation evaluation at a known oil-bearing site has been completed. Data reduction and analysis is in progress.

48. THERMODYNAMICS AND STRATEGIC MATERIALS
M. Blander, L.A. Curtiss, P.A.G. O'Hare, G.K. Johnson, V.A. Maroni, M.-L. Saboungi, J.L. Settle, R.M. Yonco
Phone: (312)-972-4548
$722,000 03-02

Experimental and theoretical studies aimed at investigating important thermodynamic, structural, and solution properties of inorganic materials including strategic and critical materials and minerals. Application of spectroscopic methods to the study of solvation and coordination chemistry of transition metals in low-melting ionic salts and other nonaqueous solvents. Exploration of new complexation methods for the dissolution of strategic and valuable metals from naturally occurring minerals and from effluent materials (e.g., fly ash) by use of spectroscopic, emf, and analytical measurements as well as theoretical models. Thermochemical measurements of the enthalpies of formation, standard entropies, and Gibbs energies of formation of strategically significant compounds that occur in both fuel and nonfuel materials and minerals. Quantum mechanical and statistical mechanical calculation of thermodynamic functions and structures of vapor complexes.

49. CHEMISTRY OF MATERIALS
R. Kumar, B. Holt, Dr. Drapcho, S. Johnson
Phone: (312)-972-4342
$515,000 03-02

Formation mechanisms of atmospheric sulfate and nitrates, and their relationship to acid precipitation chemistry. Stable oxygen isotope ratio measurements; in-situ sampling and real-time analysis and characterization of particulates; infrared spectroscopic and chemiluminescent instruments for atmospheric SO_x and NO_x species analysis; in-situ investigations of gas (SO_2, NO_x) particle reactions using an ATR-IR technique and studies of the effects of surface chemistry on sulfate and nitrate formation and neutralization mechanisms.

ARGONNE NATIONAL LABORATORY (continued)

50. ELECTROCHEMISTRY AND ENERGY SYSTEMS
M. Blander, L.A. Curtiss, G.K. Johnson, V.A. Maroni
C. A. Melendres, Z. Nagy, M.-L. Saboungi, J.L. Settle
Phone: (312)-972-4547
$603,000 03-02

Experimental electrochemical and spectrochemical measurements as well as quantum mechanical calculations to examine the mechanisms and rates of electron transfer reactions involving iron phthalocyanine and other compounds as catalysts in the cathodic reduction of O_2 at electrode surfaces. Electrochemical relaxation techniques for very fast reactions; examination of the kinetics of anodic dissolution, of incipient passivation, and of other elementary steps in corrosion; kinetics and mechanisms of inhibition. Investigation of ordered and associated solutions by a variety of experimental and theoretical techniques including emf, solubility, calorimetry, neutron diffraction, molecular dynamics, and quantum mechanical calculations. Some materials under study include chloroaluminates, ionic alloys (such as Na-Pb and Rb-Au) and metal-salt systems (such as Rb-RbCl). Spectroelectrochemical studies of polysulfide formation in aprotic media.

51. PARTICLE-SURFACE INTERACTION CHEMISTRY AND CATALYSIS
D.M. Gruen, B. Abraham, W.F. Calaway, E. Iton, A. Krauss, K. Miyano, C. Melendres, M. Mendelsohn, T. I. Morrison, M.J. Pellin, C.E. Young, G.J. Lamich
Phone: (312)-972-3513
$1,138,000 03-03

Static mode laser fluorescence spectroscopy of sputtered products from clean and adsorbate covered surfaces: a new tool for determining surface structures. Excited state and velocity distributions of sputtered atoms. Surface segregation kinetics in dilute alloy systems during energetic particle bombardment. Electronic structures of matrix isolated ligand-free transition-metal clusters. Generation of new metal-bearing shape selective medium pore zeolite catalysts useful in Fischer-Tropsch syntheses. Characterization of catalysts by EPR, FMR, PAS, and DTA techniques. Synchrotron radiation studies of catalytic materials. In-situ spectroscopic investigation of the anodic corrosion of metals. Investigation of the surface properties of polymeric monolayers on metals by nonlinear optical processes. Viscoelastic properties of monomolecular films spread on aqueous substrates.

ARGONNE NATIONAL LABORATORY (continued)

52. INTENSE PULSED NEUTRON SOURCE PROGRAM (also see page 162)
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
Phone: (312)-972-5518

$4,600,000 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-I facility is equipped with 7 insruments which are regularly scheduled for users, a low-temperature irradiation facility, 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. Aproximately 50 experiments, many involving participants in collaborative research from Universities and indusry were performed in the period Octoer 1981-March 1982, and another 60 will be scheduled for the next 6 months. Relevant Argonne research programs appear under the neutron activities of the Materials Science and Technology Division of Argonne National Laboratory.

BROOKHAVEN NATIONAL LABORATORY
Upton, Long Island, New York 11973

Corrosion Science Group - 01 -

J. R. Weeks - Phone (FTS) 666-2617 or 516-282-2617
A. N. Goland - Phone (FTS) 666-3819 or 516-282-3819

53. INTERGRANULAR STRESS CORROSION
H. S. Isaacs, K. Sieradzki, L. C. Newman.
Phone: (FTS) 666-4516 or 516-282-4516

$370,000 01-2

Mechanistic aspects of intergranular corrosion cracking and hydrogen embrittlement of iron, nickel, and copper base alloys in ambient and high temperature water. Studies of effects of heat treatment, stress, surface treatment, and sulfur compounds in solution. Electrochemical techniques include ac impedance, polarization measurements and in situ surface scanning for determining location of heterogeneities, hydrogen permeation, and dissolution in simulated crack environments. Mechanical tests include acoustic emission, stress cycling, crack growth rate measurements, constant elongation rate testing and effects of surface damage on cracking and repassivation. Surface analysis includes determination of grain boundary segregation and oxide films using scanning transmission microscopy, and x-ray photoelectron spectroscopy.

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

54. BASIC PROPERTIES OF AMORPHOUS SEMICONDUCTOR MATERIALS
P. E. Vanier, R. R. Corderman, F. J. Kampas.
Phone: (FTS) 666-3535 or 516-282-3535

$260,000 01-1

Investigations of the growth, structure, and properties of plasma-deposited thin-fim 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 x-ray absorption fine structure EXAFS. Studies of chemical bonding by infrared absorption and electron spin resonance. Measurement of photoelectronic properties and their correlation with structural and bonding characteristics.

BROOKHAVEN NATIONAL LABORATORY (continued)

55. RELATIONSHIP BETWEEN PROPERTIES AND STRUCTURES
D. O. Welch, M. Suenaga, J. Tafto, N. Higuchi.
Phone: (FTS) 666-3517 or 516-282-3517

$380,000 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.

56. PHYSICAL PROPERTIES
M. S. Pick (on leave), T. H. Metzger, S. M. Heald, D. O. Welch.
Phone: (FTS) 666-3517 or 516-282-3517

$450,000 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.

57. ELECTROCHEMICAL PROPERTIES OF INTERFACES
W. E. O'Grady.
Phone: (FTS) 666-2829 or 516-282-2829

$100,000 01-3

The role played by the structure, chemical composition, and oxidation states of the surface in electrode reactions is being studied. Electrochemical techniques combined with low energy electron diffraction, Auger electron spectroscopy, x-ray photoelectron spectroscopy, and EXAFS are being used. High surface area catalysts prepared by various techniques including ion implantation are also being investigated in an effort to bridge the gap between studies on well defined single crystals and those on microcatalyst particles.

58. PROPERTIES OF DEFECTS IN MATERIALS
C. L. Snead, Jr.
Phone: (FTS) 666-3502 or 516-282-3502

$290,000 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; enhanced diffusion applied to A15 superconductors solid-state process; 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.

LABORATORIES

BROOKHAVEN NATIONAL LABORATORY (continued)

Department of Chemistry -02-

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

59. NEUTRON SCATTERING
L. M. Corliss, J. M. Hastings, R. Thomas
Phone: (FTS)-666-4376 or (516)-282-4376

$400,000 02-1

Neutron scattering is used in this program to study the statistical mechanics of phase transitions, the dynamical properties of solids, properties and spin configurations of magnetic materials, and also crystal structures where relevant to the general program.

The strong interaction of neutrons with vibrational, rotational, and diffusive modes in crystals makes inelastic neutron scattering an excellent probe of atomic motion in solids and particularly well adapted to studies of phonons and hydrogen motion. In the case of magnetic systems one can measure the spatial distribution of magnetization and the behavior of spontaneous fluctuations, both of which are essential to understanding magnetic phase diagrams and their associated first- and second-order transitions. Because of the universal nature of critical phenomena, information gained from magnetic systems can be readily transferred to the study 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

60. MAGNETIC AND STRUCTURAL PHASE TRANSITIONS
G. Shirane, S. M. Shapiro, G. Aeppli, J. D. Axe, D. Belanger, O. Steinsvoll, J. Wicksted
Phone: (FTS) 666-3732 or 516-282-3732

3822

$1,155,000 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.

61. ELEMENTARY EXCITATIONS AND NEW TECHNIQUES
G. Shirane, L. Passell, B. H. Grier, P. Böni, C. F. Majkrzak, H. Yoshizawa
Phone: (FTS) 666-3732 or 516-282-3732

$1,400,000 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.

62. EXPERIMENTAL RESEARCH - X-RAY SCATTERING
D. E. Moncton, K. D'Amico, B. C. Frazer (on leave), L. D. Gibbs, J. B. Hastings, H. Moudden
Phone: (FTS)-666-2741 or (516)-282-2741

$ 750,000 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 and molecular orientational transitions. Extension to single crystal surfaces under ultra high vacuum conditions is in progress; study of the structure of atomic microclusters produced in nozzle beams; research and development studies of synchrotron instrumentation for NSLS experiments.

63. EXPERIMENTAL RESEARCH - LOW ENERGY - PARTICLE INVESTIGATIONS OF SOLIDS
K. G. Lynn, D. Chen (CCNY); D. Fischer, (SUNY, Stony Brook), W. J. Kossler (College of William and Mary; A. P. Mills, Jr. (Bell Labs); I. K. MacKenzie (U. Guelph, Canada); B. Nielsen, L. Roellig (CCNY); P. J. Schultz, C. L. Snead, Jr. (DAS); A. Vehanen (U. of Helsinki); M. Weber (CCNY);
Phone: (FTS)-666-3710 or (516)-282-3710

$ 630,000 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, Photo-emission, 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 μSR channel at AGS.

64. EXPERIMENTAL RESEARCH - ADVANCED MATERIALS SYNTHESIS AND CHARACTERIZATION
D. E. Cox, A. Moodenbaugh
Phone: (FTS) 666-3818/3870 or (516)-282-3818/3870

$ 365,000 02-2

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

BROOKHAVEN NATIONAL LABORATORY (continued)

65. THEORETICAL RESEARCH
V. J. Emery, P. Bak, R. Bruinsma, J. Davenport, G. J. Dienes, W. Finger, R. E. Watson, A. Zangwill
Phone: (FTS) 666-3765 or (516)-282-3765

$640,000 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.

66. PARTICLE-SOLID INTERACTIONS - RADIATION EFFECTS RESEARCH
K. G. Lynn, P. W. Levy, G. L. Snead, Jr. (DAS), K. J. Swyler (DNE)
Phone: (FTS)-666-3710 or (516)-282-3710

$ 320,000 02-4

Experimental studies of radiation-induced defects in high technology crystals in synthetic and natural minerals, in situ measurements of optical absorption and radioluminescence during electron bombardment, thermoluminescence studies in dosimeter crystals, oxides, quartz and other minerals; theory of thermoluminescence kinetics; theory of radiation; damage formation in irradiated nonmetals; radiation effects in metals, alloys and semiconductors studied by positron annihilation techniques; use of 3-MeV electron accelerator for radiation effects research. Studies on radiation damage in rock salt and other minerals encountered in waste repositories. (Supported minimally by BES.)

67. ENGINEERING PHYSICS - SURFACE SPECTROSCOPY
M. Strongin, W. Eberhardt, P. Johnson, V.J. Murgai, S. L. Weng, P. Wesner
Phone: (FTS)-666-3763 or (516)-282-3763

$ 550,000 02-5

Synchroton Radiation as a technique to study the geometrical and electronic properties of surfaces and interfaces; the use of other surface techniques such as LEED and AES, and the development of new spectroscopies such as inverse photoemission and spin polarized photoemission; techniques used to study problems including a) electronic and geometrical properties of surfaces and interfaces with special emphasis on the properties of metal overlayers, b) hydrogen on transition metals, c) organic molecules on surfaces, d) properties of catalytic surfaces, e) cooperative effects and phase transitions in adsorbate layers on surfaces, f) properties of surface compounds, g) properties of ion implanted surfaces, h) the magnetic properties of thin films.

68. LOW TEMPERATURE SURFACE PHYSICS
M. Strongin, P. Johnson, V.J. Murgai
Phone: (FTS)-666-3763 or (516)-282-3763

$ 270,000 02-5

Photoemission in disordered systems; rare gases on metal surfaces; the electronic structure of metallic clusters dispersed in rare gas solids; photoemission studies of the metal to insulator transition in granular systems; chemisorption and reactions at low temperatures; dissociation and energy transfer mechanisms on surfaces and the relationship to electronic properties.

High Flux Beam Reactor -02-

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

69. EXPERIMENTAL RESEARCH-HIGH FLUX BEAM REACTOR - OPERATIONS (also see page 158)
G. C. Kinne, D. C. Rorer, M. H. Brooks, R. C. Karol, D. G. Pitcher, M. Zukas, S. Protter, L. Junker, P. Tichler, J. Detweiler, W. Brynda
Phone: (FTS)-666-4061 or (516)-282-4061

$6,300,000 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 productions and radiation damage studies. Technical assistance is provided for experimental users, especially with regard to radiation shielding and safety review of proposed experiments. Additionally, planning and engineering assistance is provided for projects for upgrading the reactor.

BROOKHAVEN NATIONAL LABORATORY (continued)

National Synchrotron Light Source -02-

J. P. McTague: (FTS) 666-4966 or (516) 282-4966

70. EXPERIMENTAL RESEARCH - NATIONAL SYNCHROTRON LIGHT SOURCE, OPERATIONS AND DEVELOPMENT (also see page 156)

J. McTague, A. van Steenbergen, K. Batchelor, J. Galayda, J. Godel, J. Hastings, M. Howells, H. Hsieh, R. Klaffky, S. Krinsky, A. Luccio, C. Pellegrini, W. Thomlinson, G. Williams

Phone: (FTS) 666-4966 or (516) 282-4966

4635

$5,900,000 02-2

The objective of this program is to support operations and development of the National Synchrotron Light Source (NSLS). The operations aspect covers operation and maintenance of the two NSLS electron storage rings and its 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 so on. 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. While the original design has been solidly based on well developed principles of accelerator technology, this facility is the first in this country to be designed expressly for use of synchrotron radiation, and the objectives in machine performance are quite different from those of importance in high energy physics applications. An extensive R&D program is therefore necessary in order to optimize performance characteristics and also to develop new beam line instrumentation which will permit users to take full advantage of the unique research capabilities to be offered by this important new facility.

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

Materials Science Division - 01

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

71. MATERIALS SCIENCE WELDING RESEARCH
J. F. Key, H. B. Smartt, G. R. Smolik, J. W. Chan
Phone: (208)-526-8332

$400,000 01-5

Heat source/molten pool interaction studies utilizing high-speed cinematography, optical emission spectroscopy, holography, and infrared thermography to develop process models. Process parameter, material properties, solidification structure relationships. Optical metallographic microstructure characterization; solidification and heat flow modeling.

Woodhouse — 333-3888

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

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

72. EFFECT OF FLUID FLOW ON LOCALIZED CORROSION
R. C. Alkire
Phone: (217)-333-0063

$ 70,000 01-1

Transport, kinetics and convective diffusion at localized corrosion sites. Erosion, cavitation, pitting, repassivation, and transient metal salt films.

73. CENTER FOR MICROANALYSIS OF MATERIALS (also see page 174)
H. K. Birnbaum, J. A. Eades
Phone: (217)-333-8396

$210,000 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.

74. RAPID SOLIDIFICATION PROCESSING
H. L. Fraser
Phone: (217)-333-1975

$170,000 01-1

Development of rapid solidification processing of alloys with powder preparation by laser, spin and centrifugal atomization and subsequent consolidation by dynamic compaction techniques. Characterization of microstructure and measurement of properties developed by heat treatments.

75. 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 II-IV-V_2 chalcopyrite systems.

76. GRAIN GROWTH IN ALUMINA
D. S. Phillips
Phone: (217)-333-6440

$ 80,000 01-1

Transmission and analytical electron microscopy; characterization of grain boundaries in solid-state and liquid-phase sintered aluminas. Correlation of boundary mobilities in annealed thin films with these microstructures.

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (continued)

77. LASER PROCESSING OF MATERIALS SURFACES
J. M. Rigsbee and S. H. Risbud
Phone: (217)-333-6584

$ 50,000 01-1

Laser processing to modify structure, composition and physical properties of metallic and ceramic surfaces. Erosion and abrasion resistant surfaces.

78. MICROCHEMISTRY OF SOLIDS
C. W. Wert
Phone: (217)-333-1440

$ 60,000 01-1

Examination of sulfides and clays in coal by electron microscopy. Visco-elastic properties of coal and oil shale for characterization of polymer-like macromolecular nature of carbonaceous matter.

79. HYDROGEN BEHAVIOR IN BCC METALS
H. K. Birnbaum
Phone: (217)-333-1901

$190,000 01-2

Hydrogen, deuterium, tritium and helium mobility in niobium, tantalum, vanadium and nickel through classical and quantum mobility regimes. Properties and phase transitions of group Vb metal hydrides; neutron, surface, permeation and anelastic techniques. Mechanisms of hydrogen transfer across solid interfaces.

80. COUNCIL ON MATERIALS SCIENCE
D. Lazarus
Phone: (217)-333-0492

$ 60,000 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.

81. STRUCTURE, CRACKING AND CORROSION OF CERAMIC GRAIN BOUNDARIES
S. D. Brown, W. T. Petuskey, A. Zangvil
Phone: (217)-333-4766

$ 60,000 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 presures of hydrogen on strength properties. Structure of AlN-SiC solid solutions.

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (continued)

82. PHYSICAL PROPERTIES OF CERAMIC MATERIALS
W. S. Williams
Phone: (217)-333-3524

$ 95,000 01-2

Flow stress 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 limitation on flow stress. Microchemical analysis by EELS.

83. OXYGEN IN REFRACTORY BCC METALS
C. J. Altstetter
Phone: (217)-333-4985

$ 65,000 01-3

Thermodynamics and diffusion of oxygen in BCC refractory metals and dilute and concentrated alloys using solid electrolyte cells. Testing of statistical mechanical models relating diffusion and thermodynamic behavior.

84. DEVITRIFICATION BEHAVIOR IN METAL-CONTAINING SILICATE AND BOROSILICATE GLASSES
H. Chen
Phone: (217)-333-7636

$ 90,000 01-3

EXAFS, small and wide angle x-ray scattering and SEM investigation of devitrification kinetics and associated microstructural and compositional changes in silicate and borosilicate based glasses containing metal oxides.

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

$110,000 01-3

STEM, Auger and SIMS analysis of boundary conditions in electrical and structural ceramics, flux growth of ferroelectric crystals; powder preparation by molten salt synthesis and hydrothermal methods. Dielectrophoretic alignment of particles, hot-forging and hot-extrusion of ceramics; electrodes for the photoassisted electrolysis of water.

86. TRAPPING OF HYDROGEN BY SUBSTITUTIONAL SOLUTES IN REFRACTORY METAL ALLOYS
T. J. Rowland
Phone: (217)-333-1726

$ 45,000 01-3

Solute-host bonding and hydrogen distribution in refractory metal alloys containing H in solution; temperature dependence; inelastic neutron scattering, nuclear magnetic resonance, EXAFS, resistivity studies.

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (continued)

87. MICROWAVE STUDIES OF DISORDERED MATERIALS
H. J. Stapleton
Phone: (217)-333-0073
$100,000 01-3

Effects of tunnelling states and disorder in amorphous semiconductors, fast ionic conductors, and doped crystals using electron spin relaxation, ER, ENDOR, and microwave dielectric susceptibility in the 0.25-25 K range.

88. LOW TEMPERATURE STUDIES OF DEFECTS IN SOLIDS
A. C. Anderson
Phone: (217)-333-2866
$ 90,000 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.

89. PHOTOEMISSION STUDIES OF THE ELECTRONIC STRUCTURE OF SURFACES AND INTERFACES
T.-C. Chiang
Phone: (217)-333-2593
$110,000 02-2

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

90. RESPONSE OF SOLIDS TO ELECTROMAGNETIC RADIATION
J. D. Dow
Phone: (217)-333-2891 $100,000 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.

91. USE OF VERY HIGH PRESURE TO INVESTIGATE THE STRUCTURE OF MATTER
H. G. Drickamer
Phone: (217)-333-0025
$155,000 02-2

High pressure studies of the effect of tuning of energy levels and the change of macroscopic variables on atomic and molecular states and processes in condensed phases, applied to luminescence properties and optical effects at semiconductor-electrolyte interfaces.

LABORATORIES

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (continued)

92. EXCITON COLLECTION FROM ANTENNA SYSTEMS INTO ACCESSIBLE TRAPS
L. R. Faulkner
Phone: (217)-333-8306
$ 70,000 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.

93. FOREIGN ATOMS IN SUPERCONDUCTORS
D. M. Ginsberg
Phone: (217)-333-4356
$ 60,000 02-2

Use of tunnelling and critical field measurements to investigate the effect of magnetic impurities on the electronic and dynamical properties of superconductors.

94. ULTRASONIC STUDIES OF THE STRUCTURE OF MATTER
A. V. Granato
Phone: (217)-333-2639
$130,000 02-2

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

95. DEFECT AND ELECTRONIC PROPERTIES OF SOLIDS
D. Lazarus
Phone: (217)-333-0492
$ 60,000 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.

96. PROPERTIES OF CRYSTALLINE CONDENSED GASES
R. O. Simmons, V. R. Pandharipande
Phone: (217)-333-3760
$160,000 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.

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (continued)

97. NUCLEAR MAGNETIC RESONANCE IN SOLIDS
C. P. Slichter
Phone: (217)-333-3834
$155,000 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.

98. PHYSICAL PROPERTIES OF ORDERED AND DISORDERED SOLID SOLUTIONS
H. Zabel $120,000 02-2

Phone: (217)-333-2514

X-ray and neutron scattering investigations of structural, thermal and vibrational properties of alkali metal graphite-intercalation compounds; staging, dislocation and point defects, phonon dispersion, and order-disorder transformations.

LAWRENCE BERKELEY LABORATORY
University of California
Berkeley, California 94720

Materials and Molecular Research Division

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

99. Structure and Properties of Transformation Interfaces
R. Gronsky
Phone: (415) 486-5674, or FTS 451-5674

160,000 01-1

Characterization of the structure and composition of interfaces at high spatial resolution: grain boundaries, interphase boundaries, and free surfaces. Determination of the role of interfaces in solid-state reactions: structural and compositional evolution accompanying transformations.

100. Microstructure, Properties, Alloy Design: Inorganic Materials
G. Thomas
Phone: (415) 486-5656, or FTS 451-5656

540,000 01-1

Relationships between microstructure and properties; control of properties through characterization and control of structure; application of principles of strengthening and phase transformations to alloy design for mechanical (including wear) and magnetic property improvements--energy conservation; systems under investigation include ferrous alloys, dual-phase steels, rare-earth and Co-free alloys, and ceramics. Quantitative analyses of structure by electron microscopy, spectroscopy and diffraction, and high voltage, high resolution electron microscopy.

101. Solid State Phase Transformation Mechanisms
K. H. Westmacott
Phone: (415) 486-5663, or FTS 451-5663

180,000 01-1

Mechanisms of phase transformation are studied using a variety of transmission electron microscopy techniques. Specifically, the role of crystal lattice defects in precipitation reactions, vacancy-solute atom interactions in substitutional and interstitial alloy systems, segregation phenomena, impurity and minor alloy addition effects. Interrelationships between precipitation sequence, habit plane, interface structure, and orientation relations are being established for different crystal structures and compared with a developing crystallographic theory.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

102. National Center for Electron Microscopy (also see page 168)
G. Thomas, R. Gronsky, and K. H. Westmacott
Phones: (415) 486-5656, or FTS 451-5656;
(415) 486-5674, or FTS 451-5674;
(415) 486-5663, or FTS 451-5663

880,000 01-1

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

103. In-Situ Investigations of Gas-Solid Reactions by Electron Microscopy
J. W. Evans and K. H. Westmacott
Phones: (415) 642-3807;
(415) 486-5663, or FTS 451-5663

100,000 01-1

The investigation of reactions using an environmental cell in the 650 kV and 1.5 MeV high voltage electron microscopes. Emphasis is on investigation of the effect of microstructure, e.g., grain boundaries, microcracks, on the reactions between gases and solids. In-situ reductions of Fe_3O_4 to FeO by hydrogen-argon mixtures have been carried out and precipitates of FeO identified by electron diffraction and lattice fringe imaging. Characterization of commercial Fe and Cr containing oxide refractories by high voltage microscopy and energy dispersive X-ray/SEM is being performed together with in-situ reduction experiments.

104. Local Atomic Configurations in Solid Solutions
D. de Fontaine
Phone: (415) 642-8177

80,000 01-1

Study of the early stages of phase transformations in materials, primarily metallic alloys. A strong theoretical component dealing with detailed calculations of local atomic arrangements characteristic of incipient ordering and clustering. Atomic ordering studied in systems exhibiting the phenomenon of long-period superstructure formation, the theoretical tool being the cluster variation method of statistical thermodynamics and low-temperature expansion of the exact free energy, the experimental tool being high-resolution electron microscopy. Clustering, i.e., phase separation, to be studied 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 tool being transmission electron microscopy with full analytical capabilities.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

105. Collaborative Studies by TEM
A. W. Searcy
Phone: (415) 486-6062, or FTS 451-6062

40,000 01-1

Increased utilization of unique TEM instrumentation is promoted by interdisciplinary collaborations between nonelectron microscropist Divisional scientists and resident or visiting TEM specialists. Advanced high resolution, high voltage, and microanalytical techniques are applied to a variety of important scientific questions. Current studies include relationship between properties and rate of graphitization in carbon blacks, structural characterization of the graphite intercalation compound, $C_{2}{}_{0}F$, and short-range-order in Au_4Fe and its relation to magnetic properties.

106. Theoretical Problems in Alloy Design
J. W. Morris, Jr.
Phone: (415) 486-6482, or FTS 451-6482;
(415) 642-3815

505,000 01-2

The project has three objectives: to build the scientific foundation needed to approach the problem of alloy design in a systematic way, to develop systematic approaches, and to create new alloys that satisfy advanced energy needs. Specific research tasks include: (1) theory of phase transformations in solids and 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, now 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.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

107. Mechanical Properties of Ceramics
A. G. Evans
Phone: (415) 642-7347

280,000 01-2

This project is concerned with the mechanical reliability of ceramics at high temperatures. The principal research emphases are the development of a predictive capability for high temperature failure and for microstructure development during final stage sintering. Elevated temperature failure studies are concerned with the evolution of cavities and cracks at grain boundaries and within second phases. Experimental cavitation measurements are correlated with theoretical models containing the dominant microstructural variables. Final stage sintering studies are examining the processes that dictate exaggerated grain growth, retained porosity and the coarsening of the general microstructure. Theoretical descriptions are compared with microstructural measurements.

108. Environmentally Affected Crack Growth in Engineering Materials
R. O. Ritchie
Phones: (415) 486-5544, or FTS 451-5544;
(415) 642-0417

190,000 01-2

The role of microstructure and environment in influencing the subcritical and critical propagation of cracks in ferrous alloys is being examined with specific reference to i) fatigue crack growth behavior at ultralow near-threshold growth rates ($<10^{-9}$ m/cycle), ii) crack extension behavior of short flaws (comparable in size to the scale of microstructure or scale of local plasticity), and iii) the micromechanics of transgranular cleavage fracture. Research on near-threshold and short crack fatigue crack growth has been directed towards identifying mechanisms of crack closure and their role in influencing behavior. Specifically mechanisms involving cyclic plasticity, corrosion debris, meandering crack paths, viscous fluids and metallurgical phase transformations have been examined and modelled based on experimental results or bainitic, duplex ferritic/martensitic, and austenite steels.

109. High-Temperature Reactions
A. W. Searcy
Phone: 415/486-6062, or FTS 451-6062

295,000 01-3

Thermodynamics and kinetics of decomposition reactions. Thermodynamics theory for surfaces, particle shapes, and heterogeneous equilibria. Surface diffusion of vapors through porous solids. Experimental and theoretical studies of adsorption. Sintering of submicron particles. Thermodynamics of highly non-ideal carbonate solutions.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

110. Structure-Property Relationships in Semiconductor Materials
J. Washburn
Phone: (415) 486-6254, or FTS 451-6254
310,000 01-3

Structure sensitive electrical properties of semiconductor materials. Topics with close relation to state-of-the-art technology investigated jointly with the semiconductor industry and with Electrical Engineering and Computer Sciences Department at Berkeley. Use of unique high-voltage and high-resolution electron microscope facilities at Lawrence Berkeley Laboratory for the characterization of interfaces, precipitates, dislocation substructures, and radiation-induced damage. These facilities and the Rutherford scattering facility are currently being utilized for a systematic study of the crystal-to-amorphous transformation in silicon and gallium arsenide during ion implantation and to the effect of impurities and dopant elements on the kinetics of crystal growth into amorphous zones. High-resolution electron microscopy is also providing detailed information concerning the mechanisms of formation and degradation of the Cu_2S layer in CdS-Su_2S solar cells.

111. Properties and Processing of Refractory Ceramics
L. C. De Jonghe
Phone: (415) 486-6138, or FTS 451-6138
235,000 01-3

Mechanisms and kinetics of the reduction of mixed oxides by hydrogen or CO/CO_2 and study of these reactions by thermogravimetry and microanalytical and electron-optical methods. Densification and reaction in Al_2O_3-CaO powder mixtures; modeling and experiments on multiparticle sintering; densification with loading. Liquid phase and transient liquid phase densification. Rearrangement processes during sintering.

112. Structure and Electrical Properties of Composite Materials
R. H. Bragg
Phone: (415) 642-7393
125,000 01-3

Structure, electronic, and thermophysical properties of carbon materials heat treated in the range of 1000°C-3000°C. Characterization using X-ray and neutron scattering, and magnetic susceptibility, thermoelectron power, internal friction, gas permeability, C^{13} and H^1 nuclear magnetic resonance (NMR), secondary ion mass spectroscopy (SIMS), and thermogravimeter analysis (TGA) measurements.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

113. High-Temperature Oxidation and Corrosion of Materials
A. W. Searcy
Phone: (415) 486-6062, or FTS 451-6062
315,000 01-3

Mechanisms and kinetics of high-temperature corrosion reactions, in particular: the initial scale development; transport in and through scales; the scale's structure, morphology and growth mode; the mechanical integrity and adherence of the scale to the substrate; and the chemical integrity of the scale when exposed to corrosive sulfate deposits. Oxide stoichiometry changes in the presence of sulfur and transport studies in oxide solutions and their relationships to mechanisms of degradation. Active element additions to alloys and coatings to promote scale/substrate adhesion. Studies are based on thermogravimetric analyses and microscope techniques, including scanning Auger analysis.

114. Ceramic Interfaces
A. M. Glaeser
Phone: (415) 642-3821
105,000 01-3

Investigation of grain boundary migration behavior and its effects on microstructure development and stability in high-temperature oxide ceramics. Development and refinement of experimental techniques permitting the influence of solutes, pores, etc., on grain boundary migration rates to be isolated and systematically investigated. Synthesis, characterization and processing of doped and undoped alumina powders; fabrication of alumina ceramics having controlled composition and microstructure. Determination of the influence of MgO content, driving force, and temperature on migration behavior of individual grain boundaries in Al_2O_3. Experimental investigation of boundary structure transformations and their influence on microstructure development.

115. Abrasive, Erosive, and Sliding Wear of Materials
I. Finnie
Phone: (415) 642-1496
120,000 01-5

Mechanisms of abrasive, erosive and sliding wear. Simulation of microscopic wear processes by larger scale tests. Study of the effect of particle size, shape and hardness to abrasive and erosive wear. The influence of temperature and materials properties on wear rates. Correlation of wear rates to mechanical properties.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

116. Erosion of Brittle Solids
A. G. Evans
Phone: (415) 642-7347

110,000 01-5

This project is concerned with the development of a fundamental understanding of erosion and strength degradation in brittle layers and coatings subject to impact by solid particles. The principle research directions involve studies both of the damage created by the impact and indentation of individual particles and of the erosion characteristics under multiple impact conditions. The studies emphasize the influence of residual stress on the buckling and spalling of thin surface layers. The mechanics of buckling are being studied and related to crack driving forces. Relations between residual stress and spalling provide the basis for interpreting erosion data on these systems.

117. Far-Infrared Spectroscopy
P. L. Richards
Phone: (415) 642-3027

220,000 02-2

Development of improved types of far infrared detectors, mixers and spectrometers. Use of advanced infrared techniques for the measurement of: the vibrational frequencies of molecules chemically bound to metal surfaces, the infrared properties of solids with charge-density wave transitions, the far infrared spectra of organic superconductors, and the infrared photoconductivity of impurities in semiconductors.

118. Experimental Solid-State Physics and Quantum Electronics
Y. R. Shen
Phone: (415) 642-4856

255,000 02-2

The main objective of this program is to further the understanding of lasers and laser-related physics. Emphasis is on the development of linear and nonlinear optical techniques for material studies. They are being used to study current problems of interest: isotope separation, photochemistry, surface physics, and phase transitions. Recent concerted effort is in surface second harmonic generation. It is being developed to probe adsorbates at surfaces and interfaces, even between two condensed media. Theoretical and experimental investigation on various aspects of nonlinear optical interactionn with surfaces is being carried out.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

119. Excitation in Solids
C. D. Jeffries
Phone: (415) 642-3382

162,000 02-2

Study of phenomena arising when light strikes matter, in particular semiconductors like germanium: electrons are excited, leaving vacant states, or holes. At sufficient densities, excitons condense into a metallic electron-hole liquid, a novel state of matter. An unusual period doubling leading to noisy chaotic behavior is observed, which can be understood in terms of a recent universal model of approach to chaos by period doubling bifurcations. To verify this, a driven nonlinear semiconductor oscillator is being studies experimentally for a wide class of nonlinear phenomena in solids, to test the validity of universal models of routes to chaos.

120. Time-Resolved Spectroscopies in Solids
P. Y. Yu
Phone: (415) 642-8087

69,000 02-2

Application of an optical system capable of measuring adsorptivity, reflectivity, photoluminescence and light scattering spectra with time resolution of picoseconds to the study of the following phenomena: relaxation of photoexcited hot carriers via carrier-phonon interaction; decay of nonequilibrium phonon populations; temperal behavior of resonant Raman spectra and hot luminescence; trapping of carriers by deep impurity levels in semiconductors and propagation of short pulses through dispersive media.

121. Superconductivity, Superconducting Devices, and 1/f Noise
J. Clarke
Phone: (415) 642-3069

274,000 02-2

Development of Superconducting Quantum Interference Devices (SQUIDs) for measuring voltage and fluctuations in magnetic fields and magnetic field gradients, quantum noise processes in Josephson junctions and SQUIDS, operation of SQUIDs as high-frequency amplifiers. use of SQUIDs in magnetotelluric measurements of the apparent resistivity of the earth's crust, use of SQUIDS to measure magnetic field gradient fluctuations at the earth's surface. Chaos and noise in Josephson circuits. Investigation of thermoelectric effects in superconductors. Measurement of electron-phonon relaxation times in superconductors. Study of 1/f noise in Josephson junctions and SQUIDs. Dependence of 1/f noise in metal films on material properties.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

122. Theoretical Studies of the Electronic Properties of Solid Surfaces
L. M. Falicov
Phone: (415) 642-5993

70,000 02-3

Theoretical studies of: (a) the structural properties of surfaces, namely, the organization and arrangement of atomic constituents at equilibrium; (b) the 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) the electronic structure of surfaces, in particular electron states and electron densities in the neighborhood of the surface; (d) the vibronic properties of surfaces; (e) the magnetic properties of surfaces, both in magnetic solids (ferromagnetic and antiferromagnetic) or in nonmagnetic solids which may develop a magnetic surface layer; (f) the chemical--in particular the catalytic--properties of solids as they are related to the basic physical properties (a)-(e).

123. Theoretical Solid-State Physics
M. L. Cohen
Phone: (415) 642-4753

100,000 02-3

A first-principle quantum mechanical approach is used to explain and predict properties of solids. The specific techniques involve the use of pseudopotentials for electron-ion interactions, the local-density approximation for electron-electron interactions, and a momentum space total energy technique for computing structural properties. Applications to many areas in condensed matter science are made. These include: surfaces and interfaces, chemisorption, electronic band structure, optical reflectivity and photoemission, superconductivity, vibrational and structural properties, and solid-solid phase transitions.

124. Low-Temperature Properties of Materials
N. E. Phillips
Phone: (415) 642-4855

140,000 03-1

The general objective of this program is to obtain low-temperature data, particularly heat-capacity data, that contribute to an understanding of the relations between atomic properties and the macroscopic properties of materials. The materials investigated include normal and superconducting metals, superfluids, dielectric solids, and magnetic materials. Heat capacity measurements are confined to temperatures below 25 K because usually only in that region can the various contributions be reliably separated. The temperature scale for the region from 0.06 to 25 K is maintained on germanium thermometers and its relation to various "absolute" scales is well established. For temperatures from 0.06 K to the mK region, γ-ray anisotropy and nuclear susceptibility thermometers are used as primary thermometers, and various magnetic thermometers are used as working thermometers.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

125. Electrochemical Processes
C. W. Tobias
Phone: (415) 486-5208, or FTS 451-5208;
(415) 642-3764

130,000 03-1

This program is designed to advance the scientific foundations of electrochemical engineering, and to widen the range of useful applications of electrochemical transformations. Mass and charge transport in cell processes: combined influences of electrode geometry, surface potential, and ionic transport on the distribution of current on electrode profiles. Characterization of novel methods for reducing mass transfer resistance in high rate applications. Nonaqueous ionizing solvents: thermodynamic and kinetic properties of electrode reactions which are not feasible in aqueous media.

126. High-Temperature Thermodynamics
L. Brewer
Phone: (415) 486-5946, or FTS 451-5946

149,000 03-3

Characterization of the high-temperature chemical behavior of materials, particularly refractory ceramic materials, metals, and gases. The high-temperature thermodynamic properties are being determined through use of solid-electrochemical cells, solid-gas equilibria, and by X-ray and metallographic characterization of phase boundaries. The data are being used to test and improve chemical models capable of predicting the thermodynamic and elastic properties of high-temperature materials.

127. Chemistry and Materials Problems in Energy Production Technologies
D. R. Olander
Phone: (415) 642-7055

256,000 03-3

Investigation of the chemical and physical behavior of materials in the environments characteristic of energy production devices, with major emphasis on fission and fusion reactors. Experiment and study of the mechanisms involved in the high temperature behavior of uranium fuel compounds and Zircaloy cladding: transient vaporization, surface self-diffusion, high temperature corrosion and hydrogen solubility; volatile fission product release from irradiated UO_2. Molecular beam studies of chemical kinetics include hydrogen atom reaction with ceramic oxides and refractory carbides and the reactions of halogens with metals, both solid and liquid.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

128. Plasma-Enhanced Deposition of Thin Films
D. W. Hess
Phone: (415) 642-4862

49,000 03-3

This program is designed to establish scientific foundations for the rf plasma-enhanced deposition of thin films; control of chemical, magnetic, optical and electrical properties by variation of deposition parameters. Kinetic models of deposition processes as they affect solar cell fabrication, integrated circuit processing, magnetic film properties, and structure-property relations in catalyst support materials.

129. Electrochemical Phase Boundaries
R. H. Muller
Phone: (415) 486-6079, or FTS 451-6079

172,000 03-3

Advancement of the understanding of thin films and boundary layers at solid-liquid interfaces. Development and use of optical techniques for the observation of surfaces. Composition, structure and transformation of thin films, effect on chemical properties of metals and on metal deposition and dissolution reactions. Structure of adsorbed monolayers and their use for the control of phase-nucleation and growth in electrocrystallization. Determination of multilayer film structures by use of a unique self-compensating spectroscopic ellipsometer and its combination with electron spectroscopy. Investigation of boundary layers by optical interferometry; new methods to accelerate electrochemical mass transfer; control of high-rate electrolytic processes. Surface forces and thin-film interference in electrolyte films on metals.

130. Solid-State and Surface Reactions
G. A. Somorjai
Phone: (415) 642-4053; (415) 486-6160, or FTS 451-6160
(415) 486-6067, or FTS 451-6067

362,000 03-3

The research program is centered on studies of catalyzed surface reaction investigations of the atomic structure and chemical composition of solid surfaces and adsorbed monolayers. The kinetics and mechanisms of catalytic surface reactions are studied using well-characterized crystal surfaces at low and high pressures by using a combination of surface science techniques. The materials that are the focus of our studies are platinum, rhodium, iron and its compounds, rhenium, molybdenum, alkali metals and bimetallic alloys. The adsorbates and reactants are mostly hydrocarbons, oxygen, hydrogen and water. Part of the investigation is directed toward the atomic the atomic scale understanding of the structure and catalytic behavior of metal surfaces. The other part of the studies is aimed at developing new catalysts which substitute for precious metals and exhibit high rates and selectivity.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division -01- (Continued)

131. Nuclear Magnetic Resonance
A. Pines
Phones: (415) 486-6097, or FTS 451-6097;
(415) 642-1220

162,000 03-3

The primary objectives of the nuclear magnetism program are to develop methods in magnetic resonance spectroscopy and to use them to study molecular behavior in condensed phases. This demands an understanding of the interaction of nuclear spins with each other, with other degrees of freedom such as molecular translations, vibrations and rotations, and with external radiation such as light or radiofrequency sources. Novel methods developed under the program 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 are being applied to understand structure and dynamics at the molecular level in a number of materials including ferroelectrics, liquid crystals, polymers, organic crystals and zeolites. Some molecular properties change upon light excitation, and laser magnetic double resonance is being used to examine how these changes dictate the course of photochemical reactions.

132. Erosion-Corrosion Wear
A. V. Levy
Phone: (415) 486-5822, or FTS 451-5822

100,000 01-5

The combined model for prediction of erosion of ductile metals will be developed and experimentally verified. The model, developed 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, will be refined in accordance with test data. The flow test data will be generated using the LDV instrumented flow system to define the velocity, impact angle, particle size distribution, and solids loading of stream flow in various piping system geometries. The erosion data will be obtained using representative alloys used in coal conversion and combustion systems. The use of boundary layer gas to protect the surface of coal reactors from high-temperature corrosion that has analytically been proven to be feasible will be experimentally studied.

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

Materials Science Division - 01-

C. F. Cline - Phone (FTS) 532-8021 or 415-422-8021

133. HOT CORROSION STUDIES RELATED TO FOSSIL FUELS
J. J. Truhan, O. H. Krikorian
Phone: (FTS) 532-6925

$200,000 01-1

Study of mechanisms and kinetics of hot gas and molten salt corrosion of Ni- and Fe-based alloys; emphasis on reduction of the strategic element Cr in alloys without loss of corrosion resistance; corrosion analysis by thermogravimetric, linear polarization, laser raman spectroscopy, and electron microprobe techniques; alloys studied include Ni-Cr binary and Ni-Cr with separate active element additions of Hf, Ti, Y, and Nb; development of quantitative model relating Cr content to susceptibility of Ni-based alloys to corrosive media at 500-1000 C; development of mechanisms for early and middle stages of corrosion by oxidizing and sulfidizing gases and by molten salts.

134. RAPIDLY QUENCHED ALUMINUM ALLOYS
L. Tanner, L. Jacobsen
Phone: (FTS) 533-2653

$350,000 01-3

Preparation of rapidly quenched metallic alloys based on aluminum characterization and evaluation of prepared alloyws for thermal, mechanical, and corrosion resistant properties. Emphasis on high specific strength and corrosion resistance; examination of aging behavior and detailed phase relationships.

135. OPTICAL MATERIALS RESEARCH
M. J. Weber
Phone: (FTS) 532-5486

$450,000 02-2

Investigation of nonlinear optical properties of transparent materials subject to intense light beams. Intensity-dependent refractive index changes measured using time-resolved laser interferometry. Multiphoton absorption and multiphoton-induced color centers at near-ultraviolet to near-infrared wavelengths detected using photorefractive techniques. Growth and spectroscopy of new laser materials. Laser-induced fluorescence line narrowing and optical site selection spectroscopy to probe variations in local fields and electron-phonon coupling at paramagnetic ion sites in disordered solids. Dependence of spectroscopic and optical properties on materials composition. Materials include oxide and fluoride glasses and crystals.

LAWRENCE LIVERMORE NATIONAL LABORATORY (continued)

136. SURFACE PHYSICS AND CHEMISTRY OF LASER INDUCED DAMAGE
W. J. Siekhaus
Phone: (FTS) 532-6884

$280,000 02-2

Investigation of the fundamental physical and chemical process determining the thresholds for laser-induced damage of transmitting optical materials and thin-film coatings. Studies of the relation between damage thresholds of the bulk and surfaces, dependence of damage thresholds on the physical structure of surfaces, effects of adsorption of foreign atoms, surface chemical reactions, and migration of impurities. Polished crystalline and amorphous samples are cleaned by laser irradiation in a vacuum chamber and tested in situ using 1.06, 0.53 and 0.35 m laser pulses. Multiphoton induced electron, neutral atom and ion emission is monitored along with ESCA surface analysis.

137. D-T CRYOGENIC PROPERTIES
P. C. Souers, R. T. Tsugawa and E. M. Fearon
Phone: (FTS) 532-1301

$180,000 03-2

Experimental study of ultraviolet and infrared absorption peaks recently discovered in our laboratory in solid, irradiated hydrogen at temperatures below 8 K. Includes kinetics as a function of temperature and tritium content. Emission studies in the ultraviolet and visible regions also under way. Modeling of ion charge interaction with neutral hydrogen molecules is under way to elucidate the nature of the radiation defects giving rise to the spectra.

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

Materials Science and Technology Division

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

138. THE EFFECT OF SELF-IRRADIATION ON STABILITY OF CERAMIC NUCLEAR WASTE
F. W. Clinard, Jr., G. F. Hurley, D. E. Peterson, D. L. Rohr, R. B. Roof
Phone: (505)-667-5102
$277,000 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; characterization of damage effects by x-ray and electron diffraction, optical and electron microscopy, thermal conductivity, dilatometry, calorimetry, and fractography; swelling, microhardness, fracture toughness, and microcracking; role of elevated temperature during self-damage; post-irradiation annealing and recovery.

139. MECHANICAL PROPERTIES
M. G. Stout, J. J. Petrovic, P. L. Martin
Phone: (505)-667-6750
$360,000 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, brass; substructural and textural evolution with strain and strain state. Multiaxial loading brittle fracture responses of Al_2O_3, Si_3N_4, SiC, and ZrO_2; Statistical fracture theories for multiaxial loading; mixed-mode fracture of indentation-produced surface flaws and macroscopic cracks; microstructural effects on multiaxial loading brittle fracture.

140. STRUCTURAL CERAMICS
J. J. Petrovic, F. D. Gac, C. Hollabaugh, P. D. Shalek, P. L. Martin
Phone: (505)-667-5452
$226,000 01-5

Studies of fabrication-microstructure-properties interrelationships for structural ceramic materials; synthesis of dense, strong SiC and Si_3N_4 materials without the use of densification additives that can degrade elevated temperature mechanical properties; synthesis of ultrafine/ultrapure SiC and Si_3N_4 powders by RF-plasma methods; activation of powders through shock loading and irradiation treatments; consolidation of powders by colloidal chemistry and hot-pressing methods; relationships between processing and microstructure, mechanical behavior, and oxidation/corrosion response.

LOS ALAMOS NATIONAL LABORATORY (continued)

141. IMPURITY MODIFICATION OF MATERIALS: SURFACE PROPERTIES AND THIN STRUCTURAL FILMS
T. N. Taylor, C. J. Maggiore, R. W. Springer, C. T. Campbell
Phone: (505)-667-4686
$230,000 03-2

Selective modification of chemisorption properties by surface additives; relationship that electronic, structural, and compositional factors have to surface reactivity; vapor deposited metal adatoms on single crystal semimetal or oxide substrates; electron, photoelectron, and thermal 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.

Physics Division

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

142. CONDENSED MATTER RESEARCH WITH THE SNR/PSR FACILITY (also see page 164)
R. N. Silver
Phone: (505)-667-6069
$1,630,000 02-1

Neutron scattering research in condensed matter using the SNR/PSR pulsed spallation neutron source at Los Alamos. Includes studies in most areas of condensed matter; currently metal hydrides, catalysts, liquids, metallic glasses, magnetism, chemical structure, chemical spectroscopy, etc. Development of time-of-flight neutron scattering instrumentation including, currently, a filter difference spectrometer, a liquids and amorphous diffractometer, a powder diffractometer, and an electron volt spectrometer. The SNR/PSR is a national user facility for neutron scattering research in solid state physics, chemistry, materials science, biology, and polymers.

143. ULTRAHIGH-PRESSURE STUDIES OF MOLECULAR CRYSTALS
R. L. Mills, R. A. LeSar
Phone: (505)-667-4129
$200,000 02-5

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

LOS ALAMOS NATIONAL LABORATORY (continued)

144. THERMAL PHYSICS
J. C. Wheatley, G. W. Swift, A. Migliori, M. Maley, (UCSD Students: H. Haucke, J. Helffrich, Y. Maeno, T. Hofler)
Phone: (505)-667-7499
$230,000 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 in 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.

Theoretical Division

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

145. ELASTIC WAVE SCATTERING AND QUANTITATIVE FLAW AND MICROSTRUCTURE CHARACTERIZATION
R. J. Brind, J. E. Gubernatis, W. M. Visscher
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.

146. LOS ALAMOS EQUATION OF STATE LIBRARY (also see page 182)
J. Abdallah, B. I. Bennett, F. Dowell, W. F. Huebner, J. D. Johnson, D. Liberman, S. P. Lyon, K. S. Trainor
Phone: (505)-667-5751
$240,000 02-3

Maintain 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. Store data in tabular form suitable for use in realistic hydrodynamic code calculations and other applications. Distribute library programs and data to users on magnetic tapes in a universal computer format. Apply theories of solids, liquids, gases, plasmas, and mixtures to generation of EOS data. Develop new theoretical methods when existing theories and experiments are insufficient to satisfy user requirements.

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

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

147. DOE FACILITY USERS PROGRAM (also see page 172)
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.

OAK RIDGE NATIONAL LABORATORY
P. O. Box X
Oak Ridge, Tennessee 37830

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

148. 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

$550,000 01-1

Local density formalism (LDF) combined with cluster program and layer KKR program to study electronic states of surfaces and energetics such as binding energy of adsorbates, surface molecular dissociation, and chemical properties of reaction intermediates as related to catalysis; small molecular clusters, absorption of O on Al and O, S on Ni; band theory of metals, alloys and compounds, self-consistent KKR-CPA treatment of random substitutional solid solutions, residual resistivity, comparison with results of photoemission experiments, extension of theory beyond CPA; calculation of binding energies and phase stability in alloys; superconducting transition temperature and H_{C_2} and phonon line width; phonon contribution to lattice conduction; electron-phonon and electron-electron enhancement effects in metals; cohesive energy and magnetic moment of Fe.

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

$550,000 01-1

Development and use of fluorescence, 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.

150. HIGH VOLTAGE AND ANALYTICAL ELECTRON MICROSCOPY
J. Bentley, E. A. Kenik, P. S. Sklad
Phone: (615)-574-5067

$500,000 01-1

Development and application of analytical transmission microscopy and HVEM to determine the microstructure and microchemistry of solids; weak-beam dark-field 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 structural ceramics; structure of metallic glasses; standardless EELS analysis.

OAK RIDGE NATIONAL LABORATORY (continued)

151. DEFORMATION AND MECHANICAL BEHAVIOR OF STRUCTURAL MATERIALS
M. H. Yoo, J. Schneibel, C. L. White, G. F. Petersen
Phone: (615)-574-5165
$625,000 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 alloys; grain boundary cavity nucleation and growth; segregation of impurities to grain boundaries and creep cavities; dynamic recrystallization; small-angle neutron scattering studies of cavity growth during creep and fatigue in nickel and austenitic stainless steel.

152. MECHANICAL PROPERTIES OF CERAMICS
P. F. Becher, M. K. Ferber, C. J. McHargue, C. S. Yust, P. Angelini
Phone: (615)-574-5157
$500,000 01-2

Flexure strength, fracture toughness, and erosion resistance of TiB_2 as related to microcracking, slow crack growth and microstructure; wear studies of TiB_2, SiC, Al_2O_3, and transformation-toughened Al_2O_3-Zr_2O_3; slow crack growth and in situ electron microscopy studies of transformation-toughened Al_2O_3-Zr_2O_3; microhardness, indentation fracture toughness, and flexure strength of ion implanted Al_2O_3, SiC, and TiB_2.

153. 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
$750,000 01-3

Defect interactions during diffusion and during growth of surface layers; kinetics of sulfur reactions with Fe-base alloys, definition of the electronic-ionic defect structure of FeS; diffusion in sulfur-doped oxides; stress generation and relaxation in sulfide scales; sulfur attack of ion implanted Fe-base alloys. Theoretical treatment of vacancy and interstitial diffusion in compounds having high defect concentrations.

154. METASTABLE MATERIALS
C. C. Koch, A. Das Gupta, D. S. Easton, J. A. Horton, D. M. Kroeger
Phone: (615)-574-5156
$525,000 01-3

Influence of inhomogeneous deformation on structure; stability of binary and ternary metallic glasses; critical cooling rates for glass formation; preparation techniques by arc-hammer, melt spinning, and electron-beam vapor deposition; mechanical properties of metastable materials; low temperature specific heat; small-angle x-ray and TEM studies of defect structure and phase separation in Mo-Ru-B.

OAK RIDGE NATIONAL LABORATORY (continued)

155. RADIATION EFFECTS
L. K. Mansur, R. E. Clausing, K. Farrell, M. B. Lewis, N. H. Packan, L. L. Horton, E. H. Lee
Phone: (615)-574-4797
$1,400,000 01-4

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; damage simulation 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; theoretical studies of void and loop nucleation and growth, solute-defect interactions, irradiation creep, HVEM irradiations; Al, Zr, Ni and alloys, stainless steels, ferritic alloys, ceramics.

156. FUNDAMENTAL STUDIES IN WELDING
S. A. David, J. M. Vitek
Phone: (615)-574-4804
$375,000 01-5

Control of weld microstructure through control of solidification parameters; composition, distribution, and stability of microphases; microstructure of laser-produced welds; modeling of solidification processes; austenitic steels.

157. RESEARCH IN CERAMIC PROCESSING
P. F. Becher, C. B. Finch, C. J. McHargue, P. Angelini
Phone: (615)-574-5157
$325,000 01-5

Near-surface modification of Al_2O_3, SiC, Si_3N_4, and TiB_2 by ion implantation, structure determination by Rutherford backscattering and TEM, annealing; liquid phase sintering of TiB_2; sol gel powder preparation and microstructural control in transformation-toughened Al_2O_3-ZrO_2 and Al_2O_3-HfO_2; crystal growth of β'-sialon and mullite.

158. HIGH TEMPERATURE ALLOY DESIGN
C. T. Liu, J. A. Horton, A. DasGupta
Phone: (615)-574-4459
$200,000 01-5

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.

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

159. INTERATOMIC INTERACTIONS IN CONDENSED SYSTEMS
R. M. Nicklow, J. W. Cable, H. R. Child, S. Funahashi, E. Gurewitz, S. Kawarazaki, W. C. Koehler, H. A. Mook, R. M. Moon, O. A. Pringle, H. G. Smith
Phone: (615)-574-5240
$995,000 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, Tl, SmB_6, LaF_3, and intercalated graphite; magnetic excitations in amorphous materials, MnP, and Er; phase transitions in MnP, $PrAg_{1-x}Cu_x$, and random field systems; magnetic form factors of mixed-valence materials; structures of composition modulated systems.

160. PROPERTIES OF DEFECTS, SUPERCONDUCTORS, AND HYDRIDES
R. M. Moon, R. Arons, J. W. Cable, H. R. Child, W. C. Koehler, H. A. Mook, R. M. Nicklow, O. A. Pringle, H. G. Smith, G. D. Wignall
Phone: (615)-574-5234
$705,000 02-1

Elastic, inelastic, and small-angle scattering of neutrons by superconductors, metal hydrides, and defects in single crystals; lattice dynamics of α-U, A15 compounds, $PdTe_2$, metal alloys, and Na β"-alumina; proton diffusion in biological systems; magnetic structures in GdD_2 and reentrant superconductors; SANS from coal solutions, oil shale, surfactants, metal alloys, and polymer blends; kinetics of spinodal decomposition.

161. SUPPORT FOR NEUTRON USERS' PROGRAM (also see page 160)
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
$260,000 02-1

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

OAK RIDGE NATIONAL LABORATORY (continued)

162. PHYSICAL PROPERTIES OF SUPERCONDUCTORS
S. T. Sekula, Y. K. Chang, D. K. Christen, H. R. Kerchner, D. H. Lowndes, J. R. Thompson
Phone: (615)-574-6271
$405,000 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 flux-line 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.

163. PHOTOPHYSICAL PROCESSES IN SEMICONDUCTORS AND SOLAR ENERGY CONVERSION
R. F. Wood, R. B. James, G. E. Jellison, D. H. Lowndes, J. Narayan, R. D. Westbrook, C. W. White, R. T. Young
Phone: (615)-574-5781
$820,000 02-2

Effects of point defects, defect clusters, dislocations, stacking faults, and chemical impurities on electrical and optical properties of single-crystal and polycrystalline Si; fabrication of high-efficiency Si solar cells by laser techniques; thermal and laser annealing of lattice damage in Si and GaAs; laser-induced recrystallization of amorphous layers; 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; factors affecting degradation of solar cell conversion efficiency under single-sun and concentrator conditions; thin-film deposition on prepared substrates; chemical vapor deposition of Si on low-cost substrates; time-resolved optical measurements of laser-induced melting and recrystallization; picosecond laser spectroscopy, laser-induced photochemical deposition.

164. FUNDAMENTAL ASPECTS OF FRACTURE
S. M. Ohr, S.-J. Chang, T. S. Noggle, C. G. Park
Phone: (615)-574-5509
$405,000 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.

OAK RIDGE NATIONAL LABORATORY (continued)

165. SCATTERING OF SYNCHROTRON RADIATION
B. C. Larson, J. F. Barhorst, T. S. Noggle, J. Z. Tischler, C. W. White
Phone: (615)-574-5506
$130,000 02-2

Transient effects associated with pulsed-laser annealing; defect structures and defect correlations in solids; x-ray diffuse scattering; energy-resolved x-ray scattering; quasi-elastic scattering; phase transformations.

166. PHYSICAL PROPERTIES OF CERAMICS
F. A. Modine, Y. Chen, G. R. Gruzalski, T. M. Haywood, J. R. Martinelli, E. Sonder, K. L. Tsang, R. A. Weeks
Phone: (615)-574-6287
$680,000 02-2

Transition-metal carbides and nitrides and the $MgO-Al_2O_3-SiO_2$ class of refractory oxides; physical properties of materials characterized with regard to composition, defect structures, and phase segregation; studies of solid state reactions involving charge and mass transport with emphasis on materials degradation and high-temperature effects; techniques include optical and paramagnetic resonance spectroscopies, electrical properties measurements, and laser heating.

167. SOLID ELECTROLYTES AND SUPERIONIC CONDUCTIVITY
J. B. Bates, G. M. Brown, W. E. Brundage, D. Dohy, N. J. Dudney, B. C. Larson, J. C. Wang
Phone: (615)-574-6280
$385,000 02-2

Mechanisms of high ionic conductivity in the beta- and beta"-aluminas; effects of composition and crystal-growth conditions on conductivity; thermodynamics and kinetics of the hydration reactions of beta- and beta"-aluminas; effect of intercalated water on ionic conductivity; structural and dynamical properties of ionic conductors; electrical properties of beta"-alumina cermets; techniques include measurements of electrical conductivity and dielectric constant, Raman scattering, infrared absorption, neutron and x-ray diffraction, and x-ray diffuse scattering; experimental results interpreted and correlated by means of model calculations.

168. SMALL-ANGLE X-RAY SCATTERING (also see page 166)
W. C. Koehler, J. S. Lin, S. Spooner
Phone: (615)-574-5232
$130,000 02-2

Small-angle x-ray scattering of metals, 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).

OAK RIDGE NATIONAL LABORATORY (continued)

169. PREPARATION AND CHARACTERIZATION OF RESEARCH MATERIALS
L. A. Boatner, M. M. Abraham, W. E. Brundage, Y. K. Chang, L. S. Darken
Phone: (615)-574-5492

$655,000 02-2

Development of new techniques for growth of single-crystal research specimens and for preparation of advanced materials; techniques for preparation of single crystals with specified geometries; flux growth of single crystals of fast-ion conductors (β-alumina, β"-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 ($KTaO_3$, $KTa_{1-x}Nb_xO_3$) 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.

170. THEORY OF CONDENSED MATTER
J. F. Cooke, J. H. Barrett, H. L. Davis, 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

$1,200,000 02-3

Theory of laser annealing, laser-induced diffusion, and nonequilibrium solidification in semiconductors; superionic conductivity and solid electrolytes; computer simulation of radiation damage and sputtering; radiation damage analysis procedures; correlation of neutron damage with ion bombardment; radiation emitted by channeled electrons and positrons; reflection of light atoms from surfaces; surface studies with backscattered ions; development of LEED theory and interpretation of LEED data; crystallography of laser-annealed semiconductors; 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; lattice dynamics of transition metals; magnetism in transition metals; Brillouin zone integration; Heisenberg spin systems; metal-hydrogen interactions; high-temperature oxides and carbides; electronic properties of amorphous systems; lattice vibrations in disordered alloys; coherent potential approximation; vibrational properties around substitutional impurities in insulators; neutron scattering from crystals and molecular-like impurities in crystals; 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.

5508

OAK RIDGE NATIONAL LABORATORY (continued)

171. X-RAY DIFFRACTION AND ELECTRON MICROSCOPY
B. C. Larson, J. F. Barhorst, J. Narayan, T. S. Noggle, S. M. Ohr, S. Pennycook, J. Z. Tischler
Phone: (615)-574-5506

$665,000 02-4

Structure of intrinsic and induced defects in solids; transmission electron microscopy; 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; calculation of diffuse scattering from dislocation loops and solute precipitates; theory of interactions of electrons and X rays with defects in solids.

172. GASES IN METALS
R. R. Coltman, Jr., D. B. Poker, J. M. Williams
Phone: (615)-574-6263

$105,000 02-4

Interactions of light gas atoms with defects in metals; diffusivity of ion-implanted He in Ni, Cu, and stainless steels at low temperatures.

173. NATIONAL LOW-TEMPERATURE NEUTRON IRRADIATION FACILITY
R. R. Coltman, Jr., C. E. Klabunde
Phone: (615)-574-6263

$200,000 02-4

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

OAK RIDGE NATIONAL LABORATORY (continued)

174. 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

$870,000 02-5

Studies of crystallographic and electronic structure of clean and adsorbate-covered metal 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.

175. ION-BEAM ANALYSIS AND ION IMPLANTATION
B. R. Appleton, J. H. Barrett, G. M. Beardsley, R. J. Culbertson, G. C. Farlow, O. W. Holland, E. J. Kelly, C. J. McHargue, J. Narayan, T. S. Noggle, D. B. Poker, J. B. Roberto, O. E. Schow III, C. W. White, J. M. Williams, S. P. Withrow
Phone: (615)-574-6283

$825,000 02-5

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; fundamental ion damage mechanisms; 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.

OAK RIDGE NATIONAL LABORATORY (continued)

176. SURFACE MODIFICATION AND CHARACTERIZATION FACILITY AND COLLABORATIVE RESEARCH CENTER (also see page 176)
B. R. Appleton, O. E. Schow III, and C. W. White
Phone: (615)-574-6283

$370,000 02-5

SMAC facility provides 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.

177. RADIOACTIVE WASTE STORAGE
L. A. Boatner, M. M. Abraham, B. C. Sales
Phone: (615)-574-5492

$405,000 02-5

Research and development relating to use of synthetic analogs of monazite forms for disposal of commercial, U.S. defense, and transuranic wastes; growth of actinide-doped single crystals of monazites; determination of valence states and site symmetries of actinide and other impurities using electron paramagnetic resonance, x-ray, optical, and Mössbauer techniques; leaching of radioactive ions from orthophosphates and borosilicate glass under various conditions; use of molten urea process for production of orthophosphate powders with controlled particle sizes; compaction and microstructural characterization of hot-pressed or cold-pressed, sintered orthophosphate bodies; studies of heavy-particle-induced radiation effects in lanthanide orthophosphate compounds; investigations of mechanisms of borosilicate glass corrosion using Rutherford backscattering depth profiling, ion implantation, and surface analytical techniques.

178. RESEARCH AND DEVELOPMENT - ISOTOPE RESEARCH MATERIALS PREPARATION
H. L. Adair, W. S. Aaron, M. Petek, T. C. Quinby, D. W. Ramey
Phone: (615)-574-5901

$330,000 02-5

Research and development in preparation techniques involved with isotope-containing samples in the form of ultra-thin films (supported and self-supported), wires, rods, cast shapes, alloys, ceramics, cermets, distilled metals, inorganic and refractory compounds, matrix-dispersed materials, and liquids; techniques of preparation include vapor deposition, ion sputtering, rolling, chemical vapor deposition, liquid phase and conventional sintering, hot pressing, electrodeposition, molecular plating, zone refining, reactive and ordinary spray calcination, inorganic chemical methods; characterization of prepared research samples includes x-ray and electron diffraction, electron microscopy (TEM and SEM), microprobe studies, differential thermal analysis, thermal conductivity determinations, resonating crystal thickness monitoring, x-ray fluorescence, radiation counting (low geometry and absolute), and microweighing; phase diagram determinations for compounds and metals; all development efforts equivalent for stable and light and heavy radioactive materials.

OAK RIDGE NATIONAL LABORATORY (continued)
P. O. Box X
Oak Ridge, Tennessee 37830

Chemistry Division -03-

O. L. Keller — Phone (FTS) 624-4987 or 615-574-4987

179. CHEMICAL STRUCTURE OF ENERGY RELATED MATERIALS
W. R. Busing, B. K. Annis, G. M. Brown, A. H. Narten, D. W. Noid, W. E. Thiessen
Phone: (615)-574-4976

$820,000 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; small-angle neutron scattering; development of synchrotron radiation facilities. Computational methods for dynamic correction of neutron scattering intensities; improvement of statistical mechanics for understanding molecular fluids and for extrapolating their physical properties; use of intermolecular and intramolecular potentials to interpret the conformation of molecules in crystals; calculation of physical properties of crystals. Materials studied include superionic conductors for use in high-temperature batteries and fuel cells, alloys with unusual thermal properties, hydrocarbon fuels, compounds which are potential catalysts for hydrogenation and hydrogen production, water and aqueous lanthanide and actinide solutions, and silicate minerals of geochemical interest.

180. HIGH TEMPERATURE CHEMISTRY AND THERMODYNAMICS OF STRUCTURAL MATERIALS
C. E. Bamberger, J. Brynestad, G. M. Begun
Phone: (615)-574-4944

$640,000 03-2

Synthesis of high-purity structural ceramic compounds by novel reactions; emphasize exothermic homogeneous (gas-phase) and 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 particle size of 100 nm or less; reactions of BCl_3 with commercial TiB_2 to remove oxide contamination; reaction of $TiCl_2$ or $TiCl_3$ with N_2 or NH_3 to yield TiN; reaction thermodynamics and mechanisms; compaction and sintering studies.

OAK RIDGE NATIONAL LABORATORY (continued)

Chemistry Division -03-

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

F. A. Posey, A. L. Bacarella, H. R. Bronstein, G. M. Brown, E. J. Kelly, C. E. Vallet
Phone: (615)-574-5022

$700,000 03-3

Use of ion implantation/Rutherford backscattering techniques with electrochemical methods in basic studies of mechanisms of aqueous corrosion reactions occurring in localized attack of metals (titanium, vanadium, molybdenum, etc.); investigation of electrochemical and corrosion properties of precisely-defined surface alloys (Ti-Pt, Ti-Mo, Ti-V, etc.); effects of soluble redox systems [Ti(IV)/Ti(III), V(IV)/V(III)/V(II), etc.] on localized corrosion of titanium; hydrolysis and speciation 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, surface concentrations and identity of reaction intermediates, etc.).

OAK RIDGE NATIONAL LABORATORY (continued)
P. O. Box X
Oak Ridge, Tennessee 37830

Chemical Technology Division -03-

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

182. THERMODYNAMICS AND SENSITIVITY ANALYSES INVOLVING ENERGY RELATED MATERIALS
T. B. Lindemer, T. M. Besmann, C. A. Culpepper
Phone: (615)-574-6850

$262,000 03-2

Determination and modeling of phase equilibria and other thermochemical data critical to relevant energy-producing systems. Studies involve relevant subsystems in the system of elements U, Pu, Th, C, O, and specific fission products, particularly lanthanides. Second- and third-law determinations of the entropies and enthalpies of formation of relevant compounds. Modeling of nonstoichiometric actinide oxide, fluorite solid solutions. Development of generalized mathematical analyses to permit identification of those phases for which thermodynamic data must be known most precisely.

183. CHEMICAL ENGINEERING RESEARCH
D. F. Williams, C. H. Byers
Phone: (615)-574-4653

$262,000 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 interfacial properties at high pressures and temperatures. Associated thermodynamic properties measurement, correlation and development of predictive relationships. High pressure vapor-liquid equilibrium measurements.

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

184. HIGH TEMPERATURE CORROSION AND ELECTROCHEMICAL INTERACTIONS IN CERAMICS
J. L. Bates and D. D. Marchant
Phone: (509) 375-2579

$105,000 01-1

Mechanisms and kinetics of high temperature reactions of refractory metal oxides with molten silicates and gases in coal-derived environments; dissolution of oxides in liquid silicates by molecular diffusion and natural/forced convection; mass transport and diffusion studies near reaction interfaces as determined from elemental distribution using optical microscopy, SEM, quantitative electron microprobe, STEM, surface and near surface analyses; reaction studies of $MgAl_2O_4$, MgO or Al_2O_3 with liquid $CaO-Al_2O_3-SiO_2$ containing iron and magnesium. Electrochemical interactions of oxides in molten electrolytes, effect of structure on electrochemical decompositions, and evaluation of reactions between oxides, molten salts and silicates; refractory oxides include ionic and electronic conductors; effect of structure on electrochemical decompositions, and evaluation of reactions between oxides and molten salts and silicates.

185. SPUTTER DEPOSITED AMORPHOUS SEMICONDUCTORS
P. M. Martin and W. T. Pawlewicz
Phone: (509) 375-2076

$90,000 01-1

Study the effects of composition and microstructure on the electrical and optical properties and residual stress in sputtered thin film amorphous semiconductors. Develop models of reaction kinetics and film-plasma interactions occurring during the reactive sputtering process. Explore relationships between local bonding and configurations, stoichiometry and microstructure. The properties of Si_3N_4:H are currently being investigated. Measurements are being made on residual stress, bonding, phase composition and stoichiometry. Electrical property determinations include 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 include optical and infrared spectroscopy, Raman spectroscopy, in, electrical transport measurements, C-V and I-V analysis, XPS, x-ray diffraction and x-ray fluorescence.

PACIFIC NORTHWEST LABORATORY (continued)

186. EFFECT OF COAL MICROSTRUCTURE ON PROPERTIES
J. M. Lytle and L. R. Bunnell
Phone: (509) 375-2254

$90,000 01-1

Quantitative characterization of coal properties including mechanical, fracture, microstructural, and compositional; determination of the modes and mechanisms of fracture during coal comminution and the interrelationships between coal properties and fracture modes and mechanisms; determination of fracture properties of coal particles including load-displacement relationships, energy to fracture and the effect of heat, liquid, and/or sonic treatments on fracture properties; determination of the effects of both 1) energy to fracture in slow compression tests and 2) milling time in ball milling tests on the shapes of particles produced; determination of porosity, surface area, and pore size distribution as a function of ball milling time.

187. FUNDAMENTAL STUDIES OF STRESS CORROSION AND CORROSION FATIGUE MECHANISMS
R. H. Jones, M. T. Thomas, S. M. Bruemmer, D. R. Baer and M. J. Danielson
Phone: (509) 376-4276

$335,000 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. Computer modeling and experimental measurements of surface and grain boundary segregation of S, P, Sb, C, N, and O in Fe and Ni as a function of time, temperature, and bulk concentration. Relationships between grain boundary chemistry, electrochemical potential, fracture mode, ductility, crack growth rate and fracture thresholds of Fe and Ni in aqueous solutions are being studied. 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 (H_2S, Cl^-, NH_3) on the quantity and distribution of surface adsorbates is being studied by Auger Electron Spectroscopy using an in-situ straining stage.

188. OXIDATION AND CORROSION RESISTANT FINE-GRAINED MATERIALS
J. T. Prater and D. R. Baer
Phone: (509) 375-6905

$120,000 01-3

Investigate the mechanisms controlling the high-temperature corrosion of sputter-deposited fine-grained materials. Oxidation and sulfidation studies are being performed on stainless steel in CO-CO_2 and CO-CO_2-H_2S gaseous environments at 800 to 1000°C, and hot corrosion studies are being conducted on MCrAlY covered with Na_2SO_4 in an SO_2-O_2 atmosphere at 650 to 800°C. 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.

PACIFIC NORTHWEST LABORATORY (continued)

189. LEACHING OF GLASS AND CERAMICS
G. L. McVay, L. R. Pederson and D. S. Goldman
Phone: (509) 375-3672

$110,000 01-3

Mechanistic investigations of the reactions of silicate glasses and crystalline ceramics with aqueous solutions. Studies of the role of surface potential, structure, solubility, sorption, thermodynamic properties, reaction layer buildup, and chemical properties of solutions on leachability. Analytical techniques include zeta potential, radioactive and nonradioactive tracers, Rutherford backscattering spectrometry, nuclear reaction analysis, Raman scattering spectrometry, X-ray photoelectron spectroscopy, secondary ion mass spectrometry, and Fourier predictive model for glass/water interactions.

190. 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, and W. J. Weber
Phone: FTS 444-3124

$630,000 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 nickel, molybdenum, ferritics, 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, or gamma irradiation. Characterization of localized defect states in crystals and glasses 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.

191. SPUTTERING PARAMETER INFLUENCES ON MATERIAL STRUCTURE AND BEHAVIOR
R. W. Knoll, E. D. McClanahan, and W. T. Pawlewicz
Phone: (509) 375-6902

$220,000 01-5

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

PACIFIC NORTHWEST LABORATORY (continued)

192. SPUTTER-DEPOSITED COATINGS FOR OPTICAL APPLICATIONS
W. T. Pawlewicz, P. M. Martin, and D. D. Hays
Phone: (509) 375-2074

$135,000 02-2

Study of the optical properties of dielectric materials in thin-film form. Oxides, nitrides and elemental semiconductors are currently under investigation. Work includes measurement, modeling and understanding of relationships between optical properties and materials properties. Materials properties are controlled through understanding of the reactive sputtering process. Optical properties of interest are: spectral dependence of the complex refractive index; fundamental interband and lattice vibrational absorption edges; scattering; optical homogeneity, uniformity and isotropy. Related materials properties are: structure, microstructure, bonding in amorphous materials, stoichiometry, composition, purity and surface topography. Measurement techniques include transmission and reflection spectrophotometry, total integrated scattering, x-ray diffraction, Raman spectroscopy, STEM, x-ray fluorescent analysis, Nomarski microscopy, and interferometry.

193. OPTICAL AND LASER MATERIALS STUDY
J. W. Griffin and J. S. Hartman
Phone: (509) 375-2081

$125,000 02-2

Research to establish correlations between physical properties and optical losses (scattering and absorption) in optical thin films (coatings). Identify loss mechanisms; develop loss models for prediction of coating performance; provide suggestions for minimization of absorptive and scattering losses through variation of materials components, coating geometry, surface treatment and/or coating synthesis procedures. Optical diagnostic techniques include total integrated scatter (TIS), angular scattering distribution, precision spectrophotometry (reflectance and transmission), photoacoustic spectroscopy (PAS), and ellipsometry. Materials systems include single and multilayer coatings of TiO_2, ZrO_2, Ta_2O_5, Nb_2O_5, SiO_2, and Si_3N_4 on dielectric substrates.

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

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

194. STRESS CORROSION CRACKING AND ELECTROCHEMISTRY OF TRANSIENT CORROSION PROCESSES

W. H. Smyrl, R. J. Salzbrenner
Phone: (505) 844-6638 or FTS 844-6638

$140,000 01-2

Studies of crack propagation behavior of austenitic and ferritic stainless steels in molten $NaCl-AlCl_3$ environments. Importance of electrochemical reactions in cracking illustrated: Cl^- induced cracking rates shown to be directly proportional to rate of electrodissolution. Digital Faradaic Analysis used to study electrodissolution of Cr in molten $NaCl-AlCl_3$ and corrosion of Cu in aqueous solutions. Depletion of Cr observed (Auger analysis) to shallow depths under both transient and steady state conditions.

195. 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
Phone (505) 844-4309 or FTS 844-4309

$720,000 01-3

Ion implantation and ion-beam mixing are used 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 is performed by ion-beam depth-profiling, ion channeling, TEM, EPR, and optical absorption. The kinetics of transient laser/electron-beam annealing are examined by calorimetry, time-resolved reflectivity and transient conductance. In equilibrium intermetallic systems, diffusion rates, phase diagrams, and solute-trapping mechanisms are determined. New metastable crystalline and amorphous alloys are produced both by ion implantation and by transient annealing; stability bounds and microstructures are determined, and resulting improvements in mechanical and corrosion properties are measured. Methods based on ion implantation and ion beam analysis are also used to characterize the behavior of hydrogen in metals, including diffusivity, solubility, surface-barrier effects, and trapping by defects, solutes, precipitates and gas bubbles. In semiconductors, the fundamental properties of defects and impurities are determined by EPR and optical absorption following their controlled introduction by ion implantation. Laser and electron-beam annealing of silicon are investigated for the removal of implantation-doping damage, for the production of single-crystal silicon on insulators, and to elucidate fundamental aspects of rapid solidification. Refractory amorphous alloys are under study for diffusion barriers or metallization of semiconductors for elevated temperature applications.

SANDIA NATIONAL LABORATORIES (continued)

196. EROSION, WEAR AND STRESS CORROSION IN CERAMICS
T. A. Michalske, M. L. Knotek, G. A. Fisk, R. E. Cuthrell
Phone: (505) 846-3551 or FTS 846-3551
$260,000 01-5

Crack growth and fatigue properties of glasses, oxides and brittle materials; emphasis on effects of environment on crack growth and strength; chemical models for environment/strained solid interactions used to interpret fatigue effects; environments include H_2O, H_2, O_2, CH_3OH and NH_3; fatigue response measured in vacuum and other high purity environments; crack growth studies utilize direct measurement on fracture mechanics specimens; Electron Stimulated Desorption (ESD) 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 model systems (structures exhibiting high configurational strain) used to study strain-enhanced chemistry; FTIR studies of adsorbate reactions used to explore relationship between strain enhanced chemistry and stress corrosion fracture.

197. SEMICONDUCTORS FOR USE AT HIGH TEMPERATURES AND STRAINED-LAYER SUPERLATTICES
R. M. Biefeld, L. R. Dawson, I. J. Fritz, P. L. Gourley, D. R. Myers, G. C. Osbourn
Phone: (505) 844-6653 or FTS 844-6653
$300,000 01-5

Program deals with materials research in two inter-related areas of compound semiconductors: (i) semiconductors for use at high temperatures, and (ii) strained-layer superlattices. Work has a comprehensive fundamental scope and is closely integrated with modern materials growth techniques and coordinated with device physics programs to give this research technological impact. First area is motivated by a strong need for wide bandgap (Eg >1.4 eV) semiconductors for electronic devices which can operate in high temperature environments (to 500 C) such as in nuclear reactors, jet engine controls, photovoltaic concentrators, and down-hole logging in gas, oil, and geothermal wells. Second area deals with the fundamental electronic properties of the new area of strained-layer superlattices (SLS's) which is being pioneered at Sandia. SLS's represent a new class of semiconductor materials with unique and tailorable electronic and structural properties; expected to find a broad range of device applications.

SANDIA NATIONAL LABORATORIES (continued)

198. SURFACE PHYSICS RESEARCH
M. L. Knotek, D. R. Jennison, J. E. Houston, R. R. Rye, J. A. Panitz, G. L. Kellogg
Phone: (505) 844-6653 or FTS 844-6653
$310,000 02-2

Broad range of experimental and theoretical studies aimed at understanding the interaction of atoms and molecules with solid surfaces; unique local aspects of Auger Electron Spectroscopy exploited to study the variation of electronic properties during such interactions, local chemical environment of surface and adsorbed species obtained using gas-phase molecules as "absolute" standards along with theoretical analyses of the spectroscopic results; Auger applied to understand catalysis, explosive sensitivity and Si/H surface interactions. Imaging and mass spectroscopic abilities of the field-ion and field-desorption techniques developed to study the morphology of biological and other molecules. Pulsed Laser Atom Probe applied to studies of adsorption and reaction intermediate states of molecules interacting with the various planes of well defined transition metal surfaces; technique also used to observe directly adatom-adatom and adatom-defect interactions on metals.

199. ELECTRON AND PHOTON-STIMULATED DESORPTION
M. L. Knotek, G. M. Loubriel, D. R. Jennison, R. H. Stulen
Phone: (505) 844-6653 or FTS 844-6653
$275,000 02-2

Studies of metal, metal oxide, semiconductor and alkali halide surfaces as well as their interactions with H_2O, H_2, O_2 and other adsorbates using Electron- and Photon-Stimulated desorption techniques (ESD and PSD) Investigations exploit the discovery that desorption occurs by Auger decay of radiation induced core holes. Extraction of site specific, adsorbate specific electronic and structural information from both the local empty density of states (XANES) and extended x-ray absorption fine structures (EXAFS); ESD/PSD uniquely surface sensitive and sample only the uppermost layer of surface atoms. The high sensitivity to hydrogen exploited in studies of its role in catalysis, corrosion and semiconductor technology. Angle resolved photoemission and XPS using synchrotron radiation used to correlate desorption producing excitations with ground state electronic structure and many electron excitation phenomena; partial and total photoelectron yield studies to compare PSD sites to bulk sites; coincidence Auger electron/ desorbed ion measurements to determine desorption-inducing Auger final states.

SANDIA NATIONAL LABORATORIES (continued)

200. STABILITY AND CHARGE-TRANSFER PROPERTIES OF THE SOLID-LIQUID INTERFACE
M. A. Butler, D. S. Ginley
Phone: (505) 844-8863 or FTS 844-8863
$85,000 02-2

The basic charge transfer mechanisms involved in photocatalytic and photo synthetic reactions at semiconductor-electrolyte interfaces are being investigated with special attention directed at understanding the stability of these interfaces. Photoresponse measurements are used to study surface modified by ion implantation, chemisorption, or by overcoating with corrosion resistant materials. A laser scanning system has been constructed which makes photoelectrochemical measurements on semiconducting films less than 50 Å thick with a spatial resolution approaching one micron. The development of photoelectrochemical techniques for probing the solid-liquid interface will impact not only the photoelectrochemical area but should provide valuable information in the areas of catalysis, batteries and corrosion.

201. CHEMICAL VAPOR DEPOSITION RESEARCH
A. W. Johnson, W. G. Breiland, P. Ho, M. E. Coltrin
Phone: (505)-844-8782 or FTS 844-8782
$230,000 02-2

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.

SANDIA NATIONAL LABORATORIES
Livermore, California 94550

Materials Science Division - 01 -

Walter Bauer - Phone (FTS) 532-2994 or (415) 422-2994

202. GASES IN METALS
W. D. Wilson, G. J. Thomas, M. S. Daw
Phone: (FTS) 532-2264 or (415) 422-2264

$230,000 01-1

This investigation of the behavior of hydrogen and helium in metals involves joint theoretical and experimental research. The experimental program involves a variety of techniques, including electron microscopy, mechanical property measurements, and small angle neutron scattering, applied to tritiated metals and also metals implanted with helium below the damage threshold. These experiments are verifying the prediction of spontaneous lattice damage by helium which were made from fundamental calculations and how this damage influences mechanical behavior. The same theory is presently being focused on helium-dislocation interactions. A new method (Embedded Atom Method) has been developed here to calculate the cohesive energy of metals and alloys with chemically active impurities. This new method is being used to investigate the atomistic processes of fracture and the effects of hydrogen. Calculations of the trapping of hydrogen by impurities and alloying additions are also being performed.

203. MECHANISMS OF HYDROGEN EMBRITTLEMENT--EFFECTS OF GASEOUS VERSUS ELECTROCHEMICAL CHARGING
S. L. Robinson, N. R. Moody
Phone: (FTS) 532-2209 or (415) 422-2209

$110,000 01-2

A program to determine the efficacy of electrochemical charging with hydrogen to simulate gaseous environments by comparing electrochemically charged and gas charged FCC and BCC alloys. Quantify the hydrogen fugacity generated by electrochemical charging, characterize interactions of electrochemical charged hydrogen with microstructural features, determine microstructural damage resulting from charging, measure effective diffusivity for electrochemical charging.

204. PROTECTIVE BARRIERS AND COATINGS FOR COMBUSTION-RELATED MATERIALS (also see page 178)
R. E. Palmer, J. C. Hamilton, A. S. Nagelberg
Phone: (FTS) 532-3126 or (415) 422-3126

$360,000 01-1

This is a program to study corrosion/erosion mechanisms in high-temperature combustion environments, utilizing optical methods to observe the attack processes. Mechanisms of hot corrosion of ceramic turbine blade coatings by molten salt deposits are being studied in both a carefully controlled laboratory furnace and an Atmospheric Combustor Exhaust Simulator, which provides a realistic hot, particle-laden flow stream. Both facilities are instrumented for in situ Raman analysis. Corrosion by mixed gas-phase oxidants will receive increasing emphasis. In situ observations are supplemented by appropriate post-exposure analysis.

SANDIA NATIONAL LABORATORIES (continued)

205. DIAGNOSTICS FOR COMBUSTION-RELATED MATERIALS RESEARCH
R. E. Palmer, R. J. Anderson, J. C. Hamilton
Phone: (FTS) 532-3126 or (415) 422-3126

$210,000 02-5

This is a program to develop laser-based diagnostic techniques for studying corrosive/erosive processes in situ and nonintrusively at high temperature. New techniques are demonstrated on an Atmospheric Combustor Exhaust Simulator, a facility available to outside users for simulating realistic combustor exhaust environments. Techniques being developed emphasize Raman scattering and other optical techniques that can monitor surface processes and oxide layers, as well as the surrounding gaseous environment, during exposure. Complementary post-exposure techniques supplement these real-time optical diagnostics.

SOLAR ENERGY RESEARCH INSTITUTE
1617 Cole Boulevard
Golden, Colorado 80401

Solar Thermal and Materials Research Division - Materials Research Branch - 01-

G.E. Gross - Phone (FTS) 327-1228 or 303-231-1228
S.R. Bull - Phone (FTS) 327-7723 or 303-231-7723

206. SOLAR MATERIALS RESEARCH
A.W. Czanderna, P. Schissel, J.D. Webb, J.R. Pitts, T.M. Thomas
Phone: (303) 231-1240

$310,000 01-1

Degradation mechanisms and bonding at interfaces between solar materials; studies of the glass/silver, silica/silver, silver/silicon, and silver/polymer systems; silver deposition by evaporation, sputtering, and electroless deposition; polycrystalline silver films characterized for reflectance, topography, structure, and elemental composition; stability of polymer/silver interfaces, with emphasis on polycarbonate and polymethymethalcrylate; degradation in simulated solar environments; UV radiation, environmental oxidizing gases, and atmospheric pressures; interfacial catalytic and corrosion effects; diffusion, SEM, EDX, XPS, SIMS, ISS, SAM, and FT-IR, reflection absorption spectroscopy.

Solar Electric Conversion Research Division - Solid State Research Branch - 02-

S. Deb - Phone (FTS) 327-1105 or 303-231-1105
S.R. Bull - Phone (FTS) 327-7723 or 303-231-7723

207. SEMICONDUCTOR THEORY
A. Zunger
Phone: (303) 231-1172

$60,000 02-3

(1) Study of the electronic properties, structural anomalies and the interrelations between the two for ternary chalcopyrite (ABX_2, where A=Cu, B=Al, Ga, In, X=S, Se) and ternary Pnictides (ABX_2, where A=Zn, Cd, B=Si, Ge, Sn, X=P, As, Sb) semiconductors. Theoretical technique: the Mixed Basis Potential Variation band structure method. (2) Electronic structure of transition atom impurities in binary semiconductors (Si, GaP). Theoretical technique: the Quasi Band Crystal Field Green's function method. (3) Theory of optical bowing in alloys of binary semiconductors (GaP-InP). (4) Applicability of the local density functional formalism and extentions to it (the self interaction correction) for studying localized states.

SECTION B

Contract Research

(Primarily Universities)

The information on pages 75-150 was prepared by the DOE project monitor in the Division of Materials Sciences. There is considerable (about 10%) turnover in the Contract Research program and some of the projects will not be continued beyond the current contract period.

ARIZONA STATE UNIVERSITY

301. IMAGING OF SURFACES AND DEFECTS OF CRYSTALS

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

$ 97,350 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 to 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.

302. TRANSPORT IN SOLID ELECTROLYTES CONTAINING A DISPERSED SECOND PHASE

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

$ 84,917 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.

UNIVERSITY OF ARIZONA

303. ARTIFICIALLY LAYERED SUPERCONDUCTORS

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

$ 72,175 (7½ months) 02-2

An investigation of the structure of artificial metallic multilayer systems, their electronic and superconducting properties including their weak link characteristics. A major objective is to produce superlattices with higher perfection than has been yet achieved and to understand what are the important preparation parameters. The initial stage will be to fabricate layered materials with a three-gun magnetron sputtering system and use x-ray diffraction, resistance, Rutherford backscattering, TEM and other techniques such as electron tunneling and the superconducting properties to characterize the samples. A latter stage of the program will emphasize the superconducting properties of the superlattice systems and to develop weak links and microbridges with desireable properties such as an increased range of operating conditions.

BATTELLE COLUMBUS LABORATORIES

304. FAILURE OF CERAMICS FROM MULTIAXIAL STRESSES

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

$114,000 (9 months) 01-5

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

BOEING AEROSPACE COMPANY

305. X-RAY SPECTROSCOPIC INVESTIGATION OF METAMICTIZATION AND 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

$ 74,961 01-1

Detailed examination of the near neighbor site geometries of metal atoms in metamict 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 using 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.

BOSTON UNIVERSITY

306. INFRARED ABSORPTION SPECTRUM OF FREE CARRIERS IN POLAR SEMICONDUCTORS: OPTICAL ABSORPTION AND ELECTRON TRANSPORT AT HIGH FIELDS IN BULK AND LAYERED COMPOUNDS

B. Jensen - Dept. of Physics
Phone: (617)-353-2610

$ 92,640 02-3

Theoretical calculations directed at the understanding of the frequency and carrier dependence of the optical absorption coefficient and effective electron scattering time from the far to near infrared frequencies for the polar semiconductors: GaAs, InP, InAs, CdTe and ZnSe; development of a quantum theory of free carrier absorption in the presence of large magnetic or electric fields.

BOSTON UNIVERSITY (continued)

307. THEORETICAL STUDIES OF THE STATICS AND DYNAMICS OF INTERCALATION

G. Kirczenow - Dept. of Physics
Phone: (617)-353-2609

$ 69,432 02-3

Effects of charge transfer, interlayer cohesion, and in-plane and elastic interactions on the equilibrium properties and growth kinetics of the phases (or stages) of graphite intercalation compounds. Research motivated both by specific interest in quantitative comparisons of theory with experiment and by more general interest in basic physics of these materials as metastable solid state systems.

BRANDEIS UNIVERSITY

308. TWO-DIMENSIONAL COLLOIDAL SYSTEMS

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

$ 44,200 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

309. 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

$201,000 01-2

Theoretical and experimental approach to fracture behavior in metals, principally steels; near tip stress and strain fields for a moving crack in elastic - ideally plastic material under small scale yielding conditions; effect of yield surface vertices on crack tip fields; effect of carbide and martensite phase distribution on the fracture toughness of duel phase and high strength martensitic steels; cavitation as a function of plastic strain, particle size, stress triaxiality; creep cavity growth in deformation vs diffusion controlled regimes under multiaxial loading; validity of singularity describing crack tip strain fields during load transients.

310. STRAIN RATE EFFECTS IN THE DEFORMATION OF SOLIDS BY MEANS OF STRESS PULSE AND ULTRASONIC METHODS

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

$ 85,000 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 defects; metals studied - Al, Fe, Nb, Ti, Zn.

311. TIME RESOLVED FAR INFRARED SPECTROSCOPY OF EXCITONS

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

$ 75,782 02-2

High resolution time-resolved spectroscopy of excitons in semiconductors at infrared and far infrared wavelengths by tunable pulsed laser excitation on a subnanosecond time scale. GaP, ZnTe and other III-V and II-VI semiconductors.

CALIFORNIA INSTITUTE OF TECHNOLOGY

312. MELTING IN ADSORBED FILMS

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

$ 80,000 02-2

Study on melting of solid phases in adsorbed films and relationship of two-dimensional melting to three-dimensional melting. Pulsed NMR and thermodynamic measurements for methane on graphite substrates. Analysis of experimental data for physisorbed films, including the quantum systems ^{4}He and ^{3}He on graphite, in relation to current theory.

313. STUDIES OF ALLOY STRUCTURE AND PROPERTIES

W. L. Johnson - Div. of Engineering and Applied Science
Phone: (213)-356-4433

$230,000 01-1

Synthesis, structure and properties of amorphous alloys; electronic structure and superconductivity; flux pinning by crystalline precipitates; low temperature calorimetry; magnetic impurities and ordering in superconductors; local chemical and physical structure using AXD, EXAFS, X-ray Raman scattering and Mössbauer techniques; measurements of creep, ductility, yield strength and tensile strength; effects of irradiation on superconducting and mechanical properties; "point defect" structure in amorphous materials using X-ray diffraction, Mössbauer spectroscopy, internal friction and position annihilation spectroscopy.

UNIVERSITY OF CALIFORNIA/DAVIS

314. RADIATION DAMAGE AND ENVIRONMENTAL EFFECTS IN NUCLEAR WASTE STORAGE MEDIA

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

$ 93,000 01-1

Comparative evaluation of the response of nuclear waste storage glasses and candidate crystalline ceramics to irradiation is being studied over a range of temperatures in a variety of irradiation environments to determine the microstructural features enhancing deterioration and radiation instability in these materials. Effects of microstructural features, phase separation, precipitation, devitrification, particle size, and composite annealing temperatures on the properties of nuclear waste storage media. Numerical calculations of non-linear composition profiles in leached waste storage media. Estimation of damage cross sections for ionization and displacement processes in borosilicate glasses.

UNIVERSITY OF CALIFORNIA/DAVIS (continued)

315. DEFORMATION MECHANISMS AND FAILURE MODES IN SUPERPLASTICITY

A. K. Mukherjee - Dept. of Mechanical Engineering
Phone: (916)-752-0580

$ 81,000 (13 months) 01-2

Experimental study of superplastic deformation of metals, viz, microduplex austenitic stainless steels and Cu-base alloys; measurement of creep as a function of stress, temperature, strain rate, and microstructure, e.g., grain size; identification of controlling intragranular and intergranular creep mechanisms in alloys after various thermomechanical processing treatments; extension of above to cavitation behavior and superplastic forming limitations.

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

Z. A. Munir - Dept. of Mechanical Engineering
Phone: (916)-752-0559, 0580

$ 63,000 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 ceramics resulting from the decomposition of hydroxides and carbonates as a function of gas pressure, temperature, and impurities. Evaluation of changes of oxide particle shape and size as a function of sintering parameters. Morphological changes such as surface area, pore size, and overall porosity are measured and related to changes in the reversibility and rates of reactions. The role of sintering is elucidated by thermogravimetric, microscopy, and surface area measurement techniques.

UNIVERSITY OF CALIFORNIA/IRVINE

317. RAMAN SPECTROSCOPY OF MOLECULAR ADSORBATES

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

$127,000 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.

318. INTERACTION OF LOW ENERGY ELECTRONS WITH SURFACE LATTICE VIBRATIONS

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

$ 94,965 02-2

Theory of electron energy loss spectroscopy (EELS) of 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/LOS ANGELES

319. IRRADIATION-INDUCED PRECIPITATION AND SOLUTE SEGREGATION IN ALLOYS

A. J. Ardell - Materials Department
Phone: (213)-825-7011

$ 61,524 01-4

Irradiation-induced solute segregation and precipitation in Pd and Ni-base alloys; 20-750°C; proton, electron and heavy-ion irradiations to 0.25 dpa; effects of dose, dose rate, temperature, solute size misfit, damaging particle and alloy composition; voids; irradiation effects in metallic glasses; TEM, analytical electron microscopy and HVEM.

UNIVERSITY OF CALIFORNIA/SAN DIEGO

320. 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

$269,239 02-2

This is an experimental research program to investigate the coexistence of superconductivity and magnetism. The primary interest is in A-15's, ternary molybdenum chalcogenides, and other high T_c superconductors. Properties of rare earth compounds such as $ErRh_4B_4$ and $ErMo_6Se_8$ will be studied in order to understand re-entrant and coexistence phenomena. Collaborative efforts to study valance instabilities in Ce compounds and the superconductivity of graphite intercalated with potassium have been initiated. A study of the oscillatory oxidation of CO on Pt using LEED and Auger techniques and a study of some metallic thin film oxidations using electrical resistance are under way.

321. RESEARCH ON THE THERMOPHYSICAL PROPERTIES OF MATERIALS

J. C. Wheatley - Dept. of Physics
Phone: (714)-452-3325

$130,112 02-5

Studies of the science of heat engines and of cryogenic materials. The following specific areas are included: (1) Intrinsically Irreversible Engines - a refrigerating acoustically driven prototype using helium-4 as the media has been developed and will be studied, (2) The further development and analysis of a liquid propylene heat pump/prime mover, (3) Thermal convection mechanisms using helium-3 = helium-4 solutions for parameter values where chaotic behavior sets in, and (4) A study of the spin alligned isotopes of hydrogen.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA

322. RESEARCH ON PHASE TRANSFORMATIONS AND NON-EQUILIBRIUM PROCESSES

J. S. Langer - Dept. of Physics
Phone: (805)-961-3495

$ 94,053 02-3

Theory of certain non-equilibrium processes of importance in design of metallurgical materials. Theory of dendritic crystal growth. Theory of eutectic solidification with emphasis on roles played by fluctuations and instabilities. Numerical and analytic studies of theory of interfacial morphology. Kinetics of phase separation in alloy solids and multicomponent fluids.

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

$150,000 (21 months) 02-3

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

CARNEGIE INSTITUTION OF WASHINGTON

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

$ 87,000 02-2

Investigations are under way on the hydrogen isotopes, helium, neon, argon, carbon dioxide, methane and other simple gases under very high pressure. Hydrogen has been pressurized to a static pressure above 1Mbar. Laser Raman scattering studies of the molecular bonding phenomena and the elastic constants have been measured as a function of pressure to 250 kbars in hydrogen and deuterium. The Equation of State for argon has been determined to 650 kbars. Further improvement to the Diamond Anvil Cell technique is under way. The Raman and Infrared spectra of solid hydrogen will be measured to 700 kbars. Brillouin and x-ray scattering measurements on solid hydrogen and solid argon will be made to 500 kbars.

CARNEGIE-MELLON UNIVERSITY

325. CORROSION FATIGUE CRACK INITIATION UNDER PASSIVE CORROSION CONDITIONS

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

$ 89,800 01-2

Corrosion fatigue of austenitic stainless steels in aqueous solutions; correlation of dislocation characteristics and electrochemical parameters determining crack initiation under passive corrosion conditions; evaluation of the role of rupture processes, anodic dissolution, and hydrogen embrittlement; modelling fatigue lifetimes on a micromechanical basis.

CARNEGIE-MELLON UNIVERSITY (continued)

326. FUNDAMENTAL STUDIES OF EROSION AND EROSION/CORROSION FOR COAL GASIFICATION SYSTEMS

J. C. Williams - Carnegie Institute of Technology
Phone: (412)-578-2704
G. B. Sinclair - Dept. of Mechanical Engineering
Phone: (412)-578-2504

$ 65,000 01-5

Particulate erosion of ductile metals investigated for conditions of normal impact of rigid spherical particles and oblique impact of rigid cylindrical particles; strain distribution obtained based on the elastic-plastic behavior of metals at high strain rates; multiple impacts treated as quasi-fatigue cycles, leading to erosion loss described by a Coffin-Manson-type relationship; experiments with single and multiple particle impacts to measure substrate displacement, weight loss, and microstructural features such as crack paths and substructural changes; materials - Cu and its alloys; techniques - laser interferometry, electron microscopy.

CASE WESTERN RESERVE UNIVERSITY

327. COUPLED DIFFUSION PHENOMENA IN MULTICOMPONENT GLASSES AND GLASS FORMING LIQUIDS

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

$ 66,757 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 interdiffusion 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.

CASE WESTERN RESERVE UNIVERSITY (continued)

328. FUNDAMENTAL STUDIES OF STRUCTURE-PROPERTY RELATIONSHIPS IN TRANSFORMATION-TOUGHENED CERAMICS

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

$134,555 01-2

Ostwald ripening in ZrO_2 toughened Al_2O_3. Plastic deformation in two phase "single crystal" partially-stabilized ZrO_2, and in 100% tetragonal ZrO_2 polycrystals. 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.

UNIVERSITY OF CHICAGO

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

$138,157 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 include: 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 chiral fermions in lattice theories.

CLARK COLLEGE

330. STUDY OF CHARGE TRANSPORT IN THE THERMOELECTRET STATE OF SOME CERAMICS AND GLASSES

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

$ 70,000 01-3

Investigation of the mechanism of formation and decay of electrets in non-polar inorganic polycrystalline and amorphous dielectrics. Experimental characterization of electret formation with sample temperature, polarization field, and cooling rate, and of electret decay in the open and closed circuit condition. Extension of Swann-Gubkin theory by considering the non-polar part of electret polarization through the displacement of ions to account for the production of non-polar electrets. Materials of interest include $CaTiO_3$, $SrTiO_3$, $BaO \cdot 4TiO_2$, $BiTiO_3$, $(SrBi)TiO_3$, chalcogenide glasses and elemental Se. X-ray diffraction. Thermally stimulated discharge current analysis.

COLORADO SCHOOL OF MINES

331. FERROUS ALLOY METALLURGY - LIQUID LITHIUM CORROSION AND WELDING

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

$152,000 01-5

Range of austenite phase stability in Fe-Ni-Cr and Fe-Ni-Mn weld filler metals with various additions (Al, Cu, Mo, Nb, Si, Ti, W, C and N); thermal expansion coefficients for these alloys; weld metal solidification and its relation to solute partitioning; impression creep of weldments, initially of Al and of dissimilar steels; role of microchemistry and structure on weld mechanical properties; dissimilar welds in 2¼ Cr-1 Mo /316 stainless steel; gas metal arc weld strip overlay cladding process. Dissolution kinetics of austenitic stainless steels in molten Li; corrosion fatigue and embrittlement of ferritic steels in molten Li.

UNIVERSITY OF COLORADO

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

Using a variety of laser light scattering and optical microscopy techniques study lower dimensional behavior. Answer fundamental questions concerning the universality of fluid dynamical critical behavior in two dimensions. Effects of reduced dimensionality on melting of charged colloidal particle suspensions (CCPS) crystals, on supercooling of CCPS liquids and the response of CCPS crystals to transient electric fields. Dynamic critical properties of thin film fluid films. Study physics of crystalline state and liquid state colloidal particle monolayers formed on liquid surfaces and membranes.

COLUMBIA UNIVERSITY

333. DEFECT INTERACTIONS AT HIGH CONCENTRATIONS IN SOLID OXIDE ELECTROLYTES

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

$ 79,410 01-3

Interactions of defects at high concentrations in oxides that are fast-ion conductors; CeO_2 doped with Y and Sc; study of relationship between defect structure, electrical properties, and grain boundary microchemistry; relationship between simple defects that form at low concentrations and the ordering and microdomain formation observed at high concentrations; kinetics of cationic ordering. Defect energy calculations. Complex impedance plots and the "grain-boundary effect." Ordering studies as a function of ionic radius difference between M^{3+} and host cation, initially for $Zr_3Er_4O_{12}$. Analytical electron microscopy of grain boundary microchemistry. Anelastic relaxation-internal friction. Neutron scattering. Ionic thermo-current dielectric relaxation defect studies. Synchrotron EXAFS experiments on CeO_2:Y_2O_3 solid solutions at the Brookhaven National Synchrotron Light Source.

UNIVERSITY OF CONNECTICUT

334. ELECTRODE POLARIZATION STUDIES IN HOT CORROSION SYSTEMS

O. F. Devereux - Dept. of Metallurgy
Phone: (203)-486-4714

$ 73,000 01-3

Electrode polarization behavior of Ni in molten salts based on either Na_2CO_3 or FeS + Na_2S; anodic and cathodic half cell reactions identified at various O:S activities in the electrolyte; mechanisms of corrosion; kinetics of sulfidation of Fe measured in gaseous environments.

335. ENERGY TRANSFER AND NON-LINEAR OPTICAL PROPERTIES AT NEAR ULTRAVIOLET WAVELENGTHS: RARE EARTH 4f → 5d TRANSITIONS IN CRYSTALS AND GLASSES

D. Hamilton - Dept. of Physics
Phone: (203)-486-3856

$ 46,704 02-2

Investigation of non-linear optical transitions and inter-ionic energy transfer in the near UV 5d electronic states of rare earth impurity-doped crystals and glasses. Dynamic polarization spectroscopy (DPS) used as a primary technique. Other nonlinear and multiphoton spectroscopic methods also used as needed for more complete determination of the nature of the 5d orbitals.

336. THE FATIGUE BEHAVIOR OF 9- AND 12 Cr FERRITIC STEELS AT ELEVATED TEMPERATURE

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

$ 57,000 01-2

Creep-fatigue behavior of ferritic steels (9-12% Cr) related to microstructural features (grain size, carbide distribution, bainitic vs martensitic structure), oxidation resistance, fracture mechanics parameters, and fabrication (wrought vs welded condition); creep crack growth modelling for ductile alloys.

UNIVERSITY OF CONNECTICUT (continued)

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

S. Rice - Dept. of Mechanical Engineering
Phone: (203)-486-2153

$ 89,500 01-5

Experimental characterization of the formation, composition and morphology of both subsurface zones and wear debris for material 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 elasto-plastic 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.

CORNELL UNIVERSITY

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

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

$ 92,900 01-1

Characterization of the structure and electrical activity of defects in hot pressed and annealed Si bicrystals; examination of coherent and asymetric twins, and tilt and twist boundaries; relationship of boundary structure to annihilation of minority carriers and in turn to electrical activity of the Si; techniques used: HVEM, TEM, electron beam induced charge in SEM.

CORNELL UNIVERSITY (continued)

339. INITIAL STAGES OF OXIDATION OF METALS

J. M. Blakely - Dept. of Materials Science and Engineering
Phone: (607)-256-5149

$139,700 (23 months) 01-1

Relationship of structure of BeO surface films to growth kinetics and to the Be substrate morphology; effect of Ni-Fe substrate composition and surface segregation of solutes on oxide characteristics; influence of sulfur containing gases and surface modification on oxidation; transition from thin to thick oxide film; techniques used: AES, UPS, EELS, LEED.

340. MIGRATION OF GRAIN BOUNDARIES IN CERAMIC MATERIALS WITH PARTICULAR REFERENCE TO THE SINTERING PROCESS

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

$ 93,500 01-1

Study of the effect of geometry and composition of interfaces on interfacial mobility in ionic and covalent solids. Concerns include (1) misorientation between grains and boundary plane orientation, (2) geometry to interfacial dislocations and steps, (3) interfacial chemistry including local segregation and non-stoichiometry, and (4) interfacial pinning by pores or crystalline or amorphous pockets or films of a second phase. Materials of investigation include Al_2O_3, MgO, NiO, Mg-Al spinel, Si, and Ge. 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)

341. MECHANICAL PROPERTIES OF CRYSTALLINE SOLIDS

Che-Yu Li - Dept. of Materials Science and Engineering
Phone: (607)-256-4349
S. Mukherjee - Dept. of Theoretical and Applied Mechanics
Phone: (607)-256-7143

$190,000 01-2

The research includes the development of a state variable approach for the description of the mechanical properties of crystalline solids. An important objective of the work is the development of useful methods for materials testing and characterization and for stress analysis and mechanical design. Specific topics are the effects of thermal and mechanical history, deformation related phenomena, microstructure based theories, fundamental research on numerical methods and applications to complex technological problems.

342. PROBABILISTIC MODELS OF THE STRESS-RUPTURE OF COMPOSITE MATERIALS

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

$ 95,000 01-2

Modelling tensile and stress rupture strengths of fiber reinforced polymer composites based on a probabilistic statistical representation of the measured distribution of fiber strengths; development of relationships between the strength and lifetime of Kevlar fibers, fiber epoxy strands, and composite pressure vessels; influence of initial fiber breaks on composite time to failure; development of asymtotic analyses and application of these to the tensile strength of composites with different shapes and load sharing rules; extension of tensile results to 3D composites; effect of matrix viscoelasticity on creep and stress rupture for carbon, S-glass, and Kevlar fibers in polyester and epoxy matrices.

CORNELL UNIVERSITY (continued)

343. HIGH TEMPERATURE MECHANICAL BEHAVIOR OF SILICON NITRIDE

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

$117,000 (17 months) 01-2

Creep cavitation in ceramics under multiaxial loading and densification mechanisms in ceramics in the hot isostatic pressing process. In-situ measurements of densification rate of powder compacts under a variable confining pressure.

344. 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

$149,000 01-1

Investigation of grain boundary structure of metals and ceramics using TEM and x-ray diffraction; tilt boundary dislocation structure in NiO; modelling diffraction from grain boundary regions to indicate lattice dilation there.

DARTMOUTH COLLEGE

345. THE ROLE OF GRAIN SIZE ON THE BRITTLE TO DUCTILE TRANSITION OF THE STRONGLY ORDERED ALLOY Ni_3Al

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

$ 88,100 01-2

Characterization of Ni_3Al powder produced by rapid solidification; consolidation by extrusion; measurement and correlation of grain size and dislocation structure with mechanical behavior, e.g., yielding, work hardening, and creep; use of SEM to evaluate fracture morphology and AES to examine impurity segregation to grain boundaries.

UNIVERSITY OF DELAWARE

346. ANALYSES OF FAILURE MODES IN SHORT FIBER REINFORCED THERMOPLASTICS

T. W. Chou - Dept. of Mechanical and Aerospace Engineering
Phone: (302)-738-2904

$ 60,000 01-2

Calculation of physical and mechanical properties of polymers reinforced with discontinuous fibers; strength and strain hardening found for the parallel fiber case using variational and statistical methods; measurement of strength distribution of carbon and glass fibers (sometimes with prestressing) and of composites containing these; relationship of composite failure mode to fiber type and volume fraction.

UNIVERSITY OF DENVER

347. THE DETECTION OF HYDROGEN ASSISTED CRACK GROWTH

S. H. Carpenter - Dept. of Physics
Phone: (303)-753-2176

$ 72,500 01-5

Experimental investigation of H_2 induced deformation and cracking in steels; measurement of kinetics of cracking during exposure to H_2 with and without applied stress; influence of vacuum annealing on crack healing; techniques used--acoustic emission, modulus defect.

348. THERMAL EXPANSION EFFECTS IN CORDIERITE

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

$ 80,000 01-3

Effect of solid solutions of various sized ions in cordierite on thermal expansion. Solutes considered are Ge, B and P substituted on tetrahedral sites, Zn and Li substituted on octahedral sites, and alkali and alkaline earth ions interstitially in the large C-axis channels. Measurement of lattice thermal expansion coefficient on powder samples over the range from 25° to 800°C by X-ray diffraction using a Huber-Guinier high-temperature counter-based diffraction system equipped with computer control and handling of data by a Nicolet Dual L-11 system. Correlation of lattice thermal expansion with both lattice distortion and changes with X-ray diffracted intensity. Ultimate objective is to understand how changes in substitutional and interstitial lattice site occupancy and associated local bond distortions affect the lattice expansion coefficients.

EMORY UNIVERSITY

349. FAR INFRARED STUDIES OF SUPERCONDUCTING V_3Si, Nb_3Ge, AND Nb

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

$ 43,901 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 into 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 superconductors.

FLORIDA STATE UNIVERSITY

350. POLYMERS IN MECHANOCHEMICAL SYSTEMS: STRUCTURE-PROPERTY REQUIREMENTS

L. Mandelkern - Dept. of Chemistry
Phone: (904)-644-2054

$101,845 (24 months) 03-1

Studies on the influence of the lamellar, interfacial and interlamellar structures on the fundamental mechanical properties of polymers. Preparation of mixtures of molecular weight fractions of linear polyethylene to acquire a wide range of crystalline morphologies and crystallization of molecular weight fractions of linear polyethylene from a range of dilute to concentrated solutions. Studies will be performed on the mechanical behavior of a set of copolymers of varying co-unit concentration to compliment work on copolymers and branched polymers.

UNIVERSITY OF FLORIDA

351. METAL DISSOLUTION KINETICS IN ORGANIC SOLVENTS USING ROTATING RING-DISC VOLTAMMETRY

J. R. Ambrose - Dept. of Materials Science and Engineering
Phone: (904)-392-1456

$90,000 (24 months) 01-3

Characterization of electrochemistry of Ni-base binary alloys in alcohol solutions of Fe-base binary alloys in aqueous solutions; measurement of metal dissolution kinetics using rotating ring-disc voltammetry; identification of dominant processes of film formation and corrosion.

352. SYNTHESIS AND PROPERTIES OF WATER-SOLUBLE COPOLYMERS AND OTHER POLYMERS OF DEFINED STRUCTURE

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

$ 85,000 03-1

Synthesis and characterization of water-soluble polymers and other polymer analogs of interest in enhanced oil recovery. Relaxation studies will be related to various rheological properties such as shear dependent viscosity, shear degradation and drag reduction.

UNIVERSITY OF FLORIDA (continued)

353. LOW AND MODERATE TEMPERATURE OXIDATION OF ATOMICALLY 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

$110,000 01-3

Investigation of low and moderate temperature (100 K < T < 800 K) oxidation of atomically clean single and polycrystalline Ni, Cr and Ni-Cr alloys is proposed. 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.

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

J. J. Hren - Dept. of Materials Science and Engineering
Phone: (904)-392-1456

$ 76,300 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.

THE FRANKLIN INSTITUTE

355. PHYSICS OF HIGHLY ANISOTROPIC MATERIALS

Siu-Tat Chui - Physics Dept.
Phone: (302)-738-8115

$ 24,000 02-3

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

GEORGIA INSTITUTE OF TECHNOLOGY

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

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

$149,250 02-3

Theoretical studies of surface phenomena aimed toward fundamental understanding of processes which govern the properties of material surfaces. Areas included cover surface reactivity, surface crystallography, electronic and vibrational structure, dynamical processes, phase transformations and phase changes and the properties of interfaces. Surface melting and solidification have been of high current interest. Also included are studies of surface defects, heterogeneities and reaction mechanisms.

HARVARD UNIVERSITY

357. DRIFT MOBILITIES BY TIME OF FLIGHT METHODS AND TIME DEPENDENT PHOTOTRANSPORT IN THE NANOSECOND REGIME IN AMORPHOUS SEMICONDUCTORS

W. Paul - Div. of Applied Sciences
Phone: (617)-495-2853

$105,000 02-2

Transport properties of amorphous semiconductors will be determined by measurements of drift mobilities by time of flight methods and time dependent phototransport in the nanosecond regime. Correlations with characterization and physical property measurements will be made on carefully prepared samples. Computer modeling studies may be undertaken.

HARVARD UNIVERSITY (continued)

358. FUNDAMENTAL PROPERTIES OF SPIN-POLARIZED QUANTUM SYSTEMS

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

$260,000 (18 months) 02-2

A program to experimentally investigate the properties of the quantum gases of spin-polarized atomic hydrogen and deuterium. A major effort will be to attempt to reach high enough densities and low enough temperature that these unusual gases will experience Einstein-Bose Condensation. If this new form of matter is reached, the expected superfluidity of this weakly interacting gas will be sought and, if found, investigated.

UNIVERSITY OF ILLINOIS/CHICAGO CIRCLE

359. OXIDATION OF TRANSITION METALS IN CHLORINE CONTAMINATED ENVIRONMENTS

M. McNallen - Dept. of Materials Engineering
Phone: (312)-996-2436

$ 30,800 (17 months) 01-3

Experimental investigation of the oxidation of metals (Fe, Co, Ni) in mixed gas (O_2-Cl_2) environments; thermogravimetric measurement of corrosion kinetics.

UNIVERSITY OF KENTUCKY

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

P. C. Eklund - Dept. of Physics and Astronomy
Phone: (606)-257-6725

$100,035 02-2

Experimental research on graphite intercalation compounds, especially with antimony halide and alkali metal intercalates. Techniques include optical reflectance (infrared to VUV), Raman scattering, Mossbauer spectroscopy, x-ray diffraction, neutron scattering, and magnetoresistance.

361. ANISOTROPIC ELASTICITY OF COAL

P. P. Gillis - Dept. of Metallurgical Engineering and Materials Science
Phone: (606)-257-5733, 8883
A. B. Szwilski - Dept. of Civil Engineering
Phone: (606)-257-2953, 4856

$ 89,000 01-2

Investigations of the anisotropic elastic constants of coal. Static and dynamic measurements are performed and attempts to relate the results to the structure of the various coals being studied are being made. Objectives include the development of coal-sample preparation/selection procedures that lead to meaningful and reproducible research results.

362. STRUCTURAL CHARACTERIZATION OF DISPERSED METAL CATALYSTS

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

$ 94,000 (16 months) 03-3

Correlation of catalyst activity in hydrogenation reactions to the structure and morphology of the active and support phases; active phase-Ni with solutes of high oxidizing potential;support phase - SiO_2, $MgSiO_3$; techniques used: TEM, X-ray scattering.

LEHIGH UNIVERSITY

363. AN EXPERIMENTAL AND ANALYTICAL INVESTIGATION OF THE CREEP-RUPTURE PROCESS

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

$ 60,695 01-2

Experimental and modelling study of creep in austenitic stainless steels under uniaxial and multiaxial stress states; measurement of cavitation and precipitation kinetics with SANS; analysis of cavity linkage.

364. ELECTRON-OPTICAL AND MICROANALYTICAL STUDIES OF PRECIPITATION IN CERAMIC SYSTEMS

M. R. Notis - Materials Research Center
Phone: (215)-861-4225
D. B. Williams - Materials Research Center
Phone: (215)-861-4225
M. P. Harmer - Materials Research Center
Phone: (215)-861-4225

$120,000 01-1

Study of precipitation phenomena by means of analytical and high resolution electron microscopy. Phase transformation resulting in transformation toughening in ZrO_2 containing ceramics. Precipitate dissolution kinetics and transient second phase phenomena. Precipitate coarsening kinetics in NiO and CoO, and precipitation processes in mullite and ceramic glazes.

365. MECHANICS AND CHEMISTRY OF SMALL CRACKS IN CORROSION FATIGUE

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

$ 90,000 (13 months) 01-2

Experimental and theoretical study of corrosion fatigue of steels in aqueous solutions; small fatigue crack growth kinetics as a function of frequency, environment and crack length; modelling of electrochemical conditions near the crack tip and of the micromechanics of small crack growth.

LOUISIANA STATE UNIVERSITY

366. STUDIES OF SUB-MICRON DEVICES WITH EMPHASIS ON MOS SYSTEMS

R. F. O'Connell - Dept. of Physics and Astronomy
Phone: (504)-388-6835

$ 62,001 02-3

Theoretical study of electrons in quasi-two-dimensional systems, as relevant to the physics of sub-micron devices. Magneto-optical phenomena in metal-oxide-semiconductor (MOS) systems. Wigner distribution function (WDF) techniques in sub-micron device physics. Strong magnetic and electric field effects in two-dimensional systems.

UNIVERSITY OF MARYLAND

367. ADSORPTION ON METAL SURFACES

T. L. Einstein - Dept. of Physics
Phone: (301)-454-3419
R. E. Glover, III - Dept. of Physics
Phone: (301)-454-3417
R. L. Park - Dept. of Physics
Phone: (301)-454-4126

$175,000 02-2

Joint theoretical/experimental study of surface interactions which, though they involve small characteristic energies, have a significant influence on surface reactivity. Investigation of the molecular precursor state of oxygen on thin film and fully-characterized single crystal metal surfaces; identification of the physical nature of the activation barrier. Study of adatom-adatom interactions using high-resolution LEED/Auger to examine long- and short-range order of chemisorbed layers; Monte-Carlo simulations of phase diagrams will be made to obtain interaction parameters. Experimental determinations of critical exponents associated with two-dimensional phase transitions and comparison with phase-transition theory.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

368. MICROMECHANICAL MODELLING OF MICROSTRUCTURAL DAMAGE AT ELEVATED TEMPERATURE DURING CREEP OF SUPERALLOYS FOR ENERGY APPLICATIONS

A. S. Argon - Dept. of Mechanical Engineering
Phone: (617)-253-2217
F. A. McClintock - Dept. of Mechanical Engineering
Phone: (617)-253-2219

$130,000 01-2

Analysis of creep cavitation and cracking in metals--Cu, Ni-base alloys, and austenitic stainless steels; stress and strain concentrations at particles on grain boundaries modelled and their influence on local deformation and cavitation assessed; calculation of cavity growth in diffusion vs deformation controlled strain fields; relaxation processes around a macroscopic crack tip; measurement of crack growth in steels and of cavity growth kinetics under multiaxial stress states in Cu.

369. STRUCTURE AND PROPERTIES OF GRAIN BOUNDARIES

R. W. Balluffi - Dept. of Materials Science and Engineering
Phone: (617)-253-3349
P. D. Bristowe - Dept. of Materials Science and Engineering
Phone: (617)-253-3326

$311,269 01-1

Grain boundaries in metals and ceramics; experimental, theoretical and computer simulation; computer simulation of intrinsic structures of grain boundaries and grain boundary dislocations; computer simulation of the structure and energy of point defects in grain boundaries; investigation of various grain boundary models using computer simulation and physical modeling; effect of thermal energy on grain boundary structure and diffusional processes; experimental study of relationship between the energy of crystalline interfaces and their crystal misorientation; mechanisms for grain boundary migration.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

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

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

$95,000 (15 ½ 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.

371. PHYSICS AND CHEMISTRY OF PACKING FINE CERAMIC POWDERS

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

$112,000 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 colloid chemistry and mono-sized particle masses. Colloid coagulation. Surface chemistry and powder characterization. Ordering behavior of particulate assemblies. Effects of particle size distribution on slurry stability. Dispersion, packing, and sintering behavior. Generalizations controlling the presintered structure of compacts containing $\sim 10^{12}$ particles.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

372. 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 will be undertaken. Preliminary studies of these fibers has found structural, mechanical and electrical properties approaching those of graphite single crystals--superior to those of fibers formed by other techniques. Emphasis will be given to characterization by high resolution TEM studies to identify defects introduced by intercalation and implantation.

373. IRRADIATION MICROSTRUCTURES IN NUCLEAR CERAMICS FOR FUSION ENERGY AND NUCLEAR WASTE DISPOSAL

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

$134,000 01-4

Characterization of irradiation stability and radiation damage microstructures of crystalline ceramic solids and applications to radioactive waste containment. Microstructural origins of radiation-induced degradation and swelling. Irradiation responses to be investigated include point defect aggregation, phase instability, precipitation, decomposition and the crystal→glass (metamict) transformation. Accelerated irradiation is to be provided through use of fast neutrons, heavy ions, α-emitting dopants, and in certain cases (very light elements or where radiolytic damage mechanisms exist) fast electrons. Previously irradiated materials are also available for examination. Transmission electron microscopy including high-resolution structure imaging methods and scanning TEM (STEM) analytical techniques. Facilities are additionally available for examining highly-radioactive samples containing actinides. Materials to be examined include: BeO; the fluorite oxides $(Zr,Y)O_2$, PuO_2 (and the prototype fluorite CaF_2); the lithium breeder compounds Li_2O, $LiAlO_2$, Li_2ZrO_3; three non-oxide ceramics AlON, Si_3N_4, SiC; SiO_2, GeO_2 and simple silicates; the SYNROC phases $CaZrTi_2O_7$, $BaAl_2Ti_6O_{16}$; and actual PUREX waste solidified by the Sandia process.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

374. BASIC RESEARCH IN CERAMIC SYSTEMS

W. D. Kingery - Dept. of Materials Science and Engineering
Phone: (617)-253-3319
R. L. Coble - Dept. of Materials Science and Engineering
Phone: (617)-253-3318

$650,000 01-1

Electrical and optical behavior of Al_2O_3 and MgO, float zone crystal growth and zone refining of Al_2O_3, and grain boundary migration in high purity powder and bicrystals of Al_2O_3. Kinetic studies including oxygen diffusion in single crystal and deformed MgO, reaction processes and microstructure development in low temperature sub-solidus systems, influence of boundary segregation on grain boundary diffusion in MgO. Defect and grain boundary structures and interactions including non-ohmic conduction at grain boundaries in semiconducting oxides, grain boundary segregation in Al_2O_3 and MgO, electrical properties of grain boundaries in MgO, defect structure in single crystal ZnO, defect structure and complex ions at grain boundaries and surfaces, effects of silica doping on $SrTiO_3$ capacitors and ZnO varistors, and non-stoichiometry in SiC. Sintering related studies include powder preparation and sintering of Al_2O_3, grain boundary migration in alkali halides, recrystallization and creep in the W-Ni system, diffusion induced grain boundary migration and discontinuous precipitation, Co segregation at WC grain boundaries, and grain boundary: solid vapor configuration experiments. Powder preparation. Ceramic technology transfer and technology interchange.

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

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

$101,800 (9 months) 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 metallic systems and the development of improved magnetic solenoids.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

376. TRANSFORMATION PLASTICITY IN HIGH-STRENGTH MATERIALS

G. B. Olson - Dept. of Materials Science and Engineering
Phone: (617)-253-6901
I. W. Chen - Dept. of Materials Science and Engineering
Phone: (617)-253-7100
A. S. Argon - Dept. of Materials Science and Engineering
Phone: (617)-253-2217

$100,500 01-2

Development of constitutive flow relations for transformation plasticity in metals (austenitic, martensitic, and low alloy steels), ceramics (ZrO_2, HfO_2, and model alkali halides), and amorphous metals (Co-based) based on local deformation mechanisms; correlation of flow behavior with martensitic transformation kinetics, influence of stress state on transformation plasticity; deformation and microcracking processes accommodating transformation strains; techniques used--TEM, x-ray diffraction, saturation magnetization.

377. LOW TEMPERATURE AND NEUTRON PHYSICS STUDIES

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

$280,189 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 also 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.

378. A BASIC STUDY OF HEAT FLOW IN FUSION WELDING

J. Szekely - Dept. of Materials Science and Engineering
Phone: (617)-253-3236
T. Eagar - Dept. of Materials Science and Engineering
Phone: (617)-253-3229

$ 48,164 01-5

Modelling of arc welding processes; effect of spatial distribution of the heat source, e.g., point vs line, on the weld penetration and the heat affected zone width; plasma temperature and velocity profiles; weld pool shape; corroborative experiments; material-low alloy steels.

617
253
4937

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

379. FUNDAMENTAL INVESTIGATIONS OF THE OXIDATION OF ALLOYS IN MULTICOMPONENT GASEOUS ENVIRONMENTS

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

$128,400 01-3

Oxidation of Cr, Fe-Al, and Fe-Cr in gases with a range of O:S activities; differences in Cr_2O_3 formation kinetics and structure depending upon substrate crystallographic orientation; effect of CrS non-stoichiometry on oxide-sulfide boundary on stability diagrams; mechanisms controlling scale growth; comparison of corrosion behavior of conventional and rapidly solidified materials.

UNIVERSITY OF MASSACHUSETTS

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

$ 45,739 02-2

Use of ion implantation and spin quenching to form metastable A-15 and amorphous superconducting materials. Ion implantation used both 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. Current interests: Nb_3Al, implanted with B and C; Nb_3Si and Nb_3Ge, implanted with C, N, and O.

381. EROSION 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 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.

MICHIGAN STATE UNIVERSITY

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

K. N. Subramanian - Dept. of Metallurgy, Mechanics, and Materials Science
Phone: (513)-353-5197, (513)-355-5147

$ 60,653 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 TEM (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

383. 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

$118,000 (17 months) 01-2

Hydrogen embrittlement and stress corrosion cracking behavior and the influence of grain boundaries and multiaxial stresses on these phenomena. Effect of hydrogen on tensile properties and local plastic strain in bicrystals of Ni. Influence of grain boundary motion on interfacial diffusivity. Multiaxial fracture criteria for hydrogen embrittlement and stress corrosion cracking as influenced by microstructure. Influence of multiaxial loading on stress corrosion cracking in brass, and hydrogen embrittlement in Ni, Zr, and Zr alloy.

UNIVERSITY OF MICHIGAN

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

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

$ 50,000 02-2

Measurements 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, detecting orientational effects of non-spherical adsorbed molecules, and study of a variety of other surface phenomena.

385. EFFECT OF CRYSTALLIZATION OF GRAIN BOUNDARY PHASE ON THE HIGH TEMPERATURE STRENGTH OF SILICON NITRIDE CERAMICS

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

$ 79,000 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. Microstructure and phase identification in sintered and hot pressed specimens. X-ray diffraction, scanning transmission electron microscopy, electron energy loss spectroscopy, fractography analysis.

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

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

$100,000 (15 months) 01-2

Experimental investigation of intergranular stress corrosion cracking of Ni-base austenitic alloys in aqueous solutions, using Huey, Streicher, and constant extension rate tests; grain boundary composition (Cr and P level) and carbide distribution monitored with TEM and AES.

UNIVERSITY OF MINNESOTA

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

$ 83,900 01-2

Investigation of deformation-fracture-microstructure interrelationships in fatigue of Fe, Fe-Si alloys, high strength low alloy steels, and Ti-30 Mo; modelling of mechanical properties--strain rate sensitivity, flow stress and its temperature dependence, and monotonic vs cyclic loading effects; influence of microstructural features such as grain size and slip characteristics; analysis of cyclic strain hardening exponent and ductile-brittle transition temperature; modelling in terms of dislocation dynamics and fracture toughness parameters; crack closure and its effect on fatigue threshold; H_2 effects on the above; techniques used: electron channeling, SEM, TEM.

388. EXPERIMENTAL STUDY OF THE THERMODYNAMICS OF THIN FILMS AND SURFACES

A. M. Goldman - School of Physics
Phone: (612)-373-5480
E. D. Dahlberg - School of Physics
Phone: (612)-373-3358

$ 70,000 02-2

Development of a calorimeter especially suited to the study of the heat capacities of extremely thin films. Integrated circuit techniques which have been used to fabricate single-crystal silicon membrane Josephson tunneling junctions will be applied. If successful, the calorimeter will be used to study inversion layers of Si-MOS structures and phase transitions of monolayers on silicon single crystals. Auger spectroscopy and LEED used to study structure of adsorbent and adsorbate.

UNIVERSITY OF MINNESOTA (continued)

389. CORROSION RESEARCH CENTER

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

$945,000 01-1

Research and technology transfer in corrosion; multidisciplinary approach to corrosion research; theory of the double layer and electron transfer at solid-fluid interfaces; plasma-sprayed coatings; laser surface modification; adhesion of polymeric coatings; plasma-processed polymer coatings; healing processes at polymer-polymer interfaces; stress corrosion resistance of polymers in the presence of plasticizers; infrared laser-induced reactions at solid-gas interfaces; reduction and cyclic fatigue of oxide films; measurements of the oxidation state of GaAs, Fe, and Zn alloys with Auger electron and X-ray spectroscopies and other electrochemical methods; high temperature oxidation of Fe-Cr-Al alloys in gases with a range of O:S activities; hot corrosion of oxide scales in molten sulfates.

UNIVERSITY OF MISSOURI/COLUMBIA

390. DEVELOPMENT AND CHARACTERIZATION OF HIGH TEMPERATURE ELECTRICALLY CONDUCTING OXIDES

H. E. Anderson - Dept. of Ceramic Engineering
Phone: (314)-341-4886, 4401

$112,000 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 specimen preparation, thermogravimetric measurements, X-ray diffraction, transmission electron microscopy, and magnetic susceptibility, Hall, conductivity, and Seebeck measurements.

UNIVERSITY OF MISSOURI/COLUMBIA (continued)

391. INELASTIC SCATTERING IN CONDENSED MATTER WITH HIGH INTENSITY MÖSSBAUER 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, Purdue University
Phone: (317)-494-3031

$175,000 (19 months) 02-2

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

UNIVERSITY OF MISSOURI/KANSAS CITY

392. ELECTRONIC PROPERTIES OF AMORPHOUS SILICON DIOXIDE AND METALLIC IONS IN SILICATE GLASSES

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

$ 40,000 01-1

Theoretical study of the electronic properties of crystalline SiO_2, Si_3N_4, silicon oxynitrides, alkali silicates, amorphous SiO_2, and silicate glasses containing impurities such as hydrogen, hydroxl, alkali, and transition metal ions by the OLCAO method. Results concern electron density of states, energy band gaps, chemical bonding, charge transfer and charge density distribution, local density of states, optical absorptions, etc. Nature and location of impurity states of various ions in the silicate glass network, and impurity-host interactions. Comparison of calculated local density of states with UPS and XPS measurements underway at Argonne National Laboratory. Development of a direct-space self-consistent field method for the electronic structure calculation within the LCAO framework.

NATIONAL BUREAU OF STANDARDS

393. 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.

UNIVERSITY OF NEVADA

394. PHOTOPHYSICAL STUDIES OF TRIPLET EXCITON PROCESSES IN PURE POLYMER FILMS

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

$ 78,347 03-1

Evaluate photophysical rate constants relevant to solid films of poly (N-vinylcarbazole) and related to photon collection and energy transmission.

NEW MEXICO INSTITUTE OF MINING AND TECHNOLOGY

395. 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

396. RADIATION EFFECTS AND ANNEALING KINETICS IN CRYSTALLINE SILICATES, PHOSPHATES, AND COMPLEX Nb-Ta-Ti OXIDES

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

$ 95,000 01-1

Comparative study of the properties of selected metamict minerals and synthetic irradiated phases of similar composition. In order to correlate radiation effects in synthetic phases (e.g., fission track formation and fading) with the process of metamictization, the following properties of metamict minerals will be examined: (a) refractive index birefringence and density (b) microstructure, (c) annealing kinetics, and (d) leach behavior. One of the major effects of this part of the study will be the determination of the structure of the metamict state by the use of electron microscopy and extended X-ray absorption fine structure spectroscopy. Annealing and recrystallization kinetics of the metamict and partially metamict phases.

CITY UNIVERSITY OF NEW YORK/BROOKLYN COLLEGE

397. OPTICAL AND ELECTROCHEMICAL INVESTIGATION OF RUTHENIUM AND IRIDIUM AND THEIR OXIDES IN RELATION TO THEIR ELECTROCATALYTIC ACTIVITY

F. H. Pollak - Dept. of Physics
Phone: (212)-780-5356

$164,000 (18 months) 03-3

Studies of factors affecting behavior of single-crystal Ru and Ir oxides as electrocatalysts for the O_2 evolution reaction. Determination of electronic energy levels and density of states from optical and u.v. photoemission, Raman and infrared spectroscopy. In situ electrochemical and combined electrochemical-optical measurements.

CITY UNIVERSITY OF NEW YORK/CITY COLLEGE

398. ELECTRONIC AND OPTICAL PROPERTIES OF DISORDERED SYSTEMS

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

$ 85,000 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.

CITY UNIVERSITY OF NEW YORK/CITY COLLEGE (continued)

399. STUDY OF FORMATION OF SURFACE FILMS: CRITICAL CONDITIONS FOR GROWTH

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

$ 42,529 01-5

Experimental studies of the critical conditions for growth of surface films in a UHV reaction system with pressure of the gaseous reactants and substrate temperature as the primary variables. Principal systems under investigation consist of (1) silicon nitride and oxynitride films formed via reaction of NO with Si(111) and Si(100), (2) silicon carbide formed via the interaction of C_2F_4 or $C_2H_2F_2$ with Si(111) and Si(100) and (3) silicon carbide formed via the CH_4 + Si reaction. Analytical techniques include scanning electron microscopy, Auger electron spectroscopy, X-ray photoemission spectroscopy at the BNL-NSLS.

POLYTECHNIC INSTITUTE OF NEW YORK

400. PHOTOEMISSION STUDIES OF f-ELECTRON SYSTEMS: MANY BODY EFFECTS

R. D. Parks - Dept. of Physics
Phone: (212)-643-2070

$ 75,000 02-2

Photoemission studies of rare earth systems, particularly intermetallic compounds, aimed at understanding electronic phenomena underlying the 4f instabilities in mixed valent and Kondo lattice systems. Synchrotron radiation is a major experimental tool in these studies.

STATE UNIVERSITY OF NEW YORK/STONY BROOK

401. CONSTRUCTION AND MAINTENANCE OF SUNY FACILITIES AT THE NATIONAL SYNCHROTRON LIGHT SOURCE (Several Institutions Involved)

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

$300,000 02-2

An X-ray beam line is being built and instrumented at the National Synchrotron Light Source (NSLS) under the auspices of this Participating Research Team (PRT). This PRT represents campuses at Albany, Buffalo, Stony Brook, Cortland, and Alfred. This line will include facilities for high resolution crystallography, surface physics, small angle scattering, and EXAFS.

STATE UNIVERSITY OF NEW YORK/STONY BROOK (continued)

402. SYNCHROTRON TOPOGRAPHIC PROJECT PARTICIPATING RESEARCH TEAM (Several Institutions Involved)

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

$460,000 01-1

Conclusion of initial phase design and construction of beam-line X-19 at the National Synchrotron Light Source so that a basic work station furnished with an operational White Beam Camera (WBC) and a Multiple Crystal Camera (MCC) for monochromatic topography. This Synchrotron Topography Project for the NSLS facility beam-line will develop a research effort on a range of scientific problems where Synchrotron Topography can make unique contributions. Absorption edge contour and synchrotron x-ray fractography to characterize individual dislocations and local strain fields. Scientific work encompasses characterization of Si chips and metal-silicide thin films, local strain studies in CdS after pressure quenching, studies on fracture in tungsten bi-crystals and of the role of grain boundaries in high temperature failure, thermal decomposition studies in inorganic crystals, investigations of fundamental fracture mechanisms of semi-brittle materials, and studies of the interaction of acoustic waves with microstructure and defects in structural and electronic materials.

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

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

$242,236 (20 months) 02-2

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

STATE UNIVERSITY OF NEW YORK/STONY BROOK (continued)

404. CHEMISORPTION THEORY: ADSORPTION ON COPPER-NICKEL ALLOYS AND TITANIUM SURFACE EMBRITTLEMENT

J. L. Whitten - Dept. of Chemistry
Phone: (516)-246-6068, 5050

$ 90,000 03-3

An embedding theory for treating chemisorption on metals extended and applied to systems involving Ti, Cu, Ni and Cu/Ni alloy and H_2, H, Co, C, and coabsorbed H and C adsorbates. Emphasis on the energetics of adsorption as a function of surface site and composition to determine the reactivity of adsorbed species.

NORTH CAROLINA AGRICULTURAL AND TECHNICAL UNIVERSITY

405. EFFECT OF FATIGUE AND THERMAL LOADS ON SILICON CARBIDE 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

$ 50,000 01-5

Structural characterization of SiC/glass matrix fibers before, during, and after tension and thermal fatigue testing from room temperature to 650°C at a stress amplitude ratio of 0.1 and a frequency of 10Hz. Radiographic examination for delaminations, debonding, fiber breakage, etc. Optical and scanning electron microscopy microstructural characterization.

NORTH CAROLINA STATE UNIVERSITY

406. DEVELOPMENT OF AN X-RAY BEAM LINE AT THE NSLS FOR STUDIES IN MATERIAL SCIENCE USING X-RAY ABSORPTION SPECTROSCOPY (Several Institutions Involved)

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

$275,000 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 will cover the energy range from 1-20 KeV and include provisions for transmission EXAFS, fluorescence EXAFS, surface EXAFS and X-ray absorption studies. Materials science research to be addressed includes areas of metallurgy, corrosion, amorphous materials, catalysis, surface science, electrochemistry and magnetic properties.

407. THE EFFECT OF MICROSTRUCTURE OF SOLID-PARTICLE EROSION IN MULTIPHASE MATERIALS

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

$ 90,000 (13 months) 01-5

Correlation of erosion rates in multiphase alloys with constituent phase properties, morphology, and distribution; systems to be studied include ductile-brittle mixtures (e.g., Al-Si, Co-Al, Ni-Al_2O_3) and brittle materials (e.g., oxides); modelling of erosion to derive constitutive laws; computer simulation.

NORTHEASTERN UNIVERSITY

408. 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

$ 81,000 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

409. DEFECT CLUSTERS AND ELECTRICAL PROPERTIES IN TRANSITION METAL MONOXIDES

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

$112,240 (10 months) 01-1

Measurements of defect structure and electrical properties and quantum theoretical calculations for multicomponent transition metal oxides. Electrical measurements and analysis based on Arrhenius plots of conductivity at constant Seebeck coefficient for MnO and NiO. Valence studies via X-ray absorption edge, TEM critical voltage technique, and photoelectron spectroscopy. Defect interaction studies in MnO and CoO via X-ray (synchrotron at the BNL NSLS) and pulsed neutron scattering (at the ANL IPNS). Preliminary electrical and structural studies of ScO and CrO. Self-consistent-field local density theory calculations for the electronic structure associated with isolated vacancies and defect clusters. Use of an energy band code based on the Linearized Muffin Tin Scheme to calculate and compare band structures, Fermi surfaces, and transport properties with experimental studies.

NORTHWESTERN UNIVERSITY (continued)

410. 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

Using an ultralow temperature neutron diffraction facility at Argonne National Laboratory, nuclear magnetic ordering phenomena will be investigated. The primary effort will be a determination of the nature of the nuclear ordering in solid helium-3, a result of fundamental importance. The program will also investigate the ordering of nuclear spins in metals such as $PrCu_6$.

411. EFFECT ON POINT DEFECTS ON MECHANICAL PROPERTIES OF METALS

M. Meshii - Dept. of Materials Science
Phone: (312)-492-3213

$ 87,000 01-2

Experimental and analytical investigation of low temperature flow behavior of Nb; influence of crystallographic orientation and interstitial atoms on deformation by primary vs anomalous slip; H_2 effects on dislocation motion, low temperature on hardening and softening, as well as on fracture of Fe by intergranular quasi-cleavage or microvoid coalescence; trapping of H_2 and S impurities.

412. 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

$ 63,275 01-2

Investigation of deformation, failure, and microstructural stability during creep and creep fatigue in low alloy ferritic steels; TEM and SANS characterization of strain and thermal induced microstructural modifications, e.g., carbide precipitation, cavity formation; influence of prestrain on residual stress and hydrogen attack.

NORTHWESTERN UNIVERSITY (continued)

413. 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 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 transient spectroscopy, Hall measurements, photocapacitance, and spectrally resolved photocurrent measurements.

414. BASIC RESEARCH ON CERAMIC MATERIALS FOR ENERGY STORAGE AND CONVERSION SYSTEMS

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

$ 71,500 01-1

Investigation of factors affecting electronic and mass transport behavior in solid electrolyte and electrode materials; study of the effect of a dispersed second (non-soluble) phase on ionic transport in solid electrolytes; synthesis and characterization of new materials which may have application as solid electrodes or electrolytes in energy storage or conversion; and optimization of the factors affecting the fabrication and ion transport properties of dense polycrystalline specimens of new solid electrolyte and electrode materials. Techniques employed include ac conductivity, dc polarization measurements, tracer diffusion, dielectric loss, ion thermal current measurements, Raman spectroscopy, NMR line-narrowing and pulsed field gradient experiments, chemical preparation and crystal growth of selected electrolyte materials. Materials under investigation include mixed ammonium and hydrogen beta"-aluminas, their deuterated counterparts, and analogous gallates; Li_2O-LiCl-B_2O_3 and Li_2O-LiF-B_2O_3 glasses; and LiI-silica composites.

Gil Stein - 312-492-5284

UNIVERSITY OF NOTRE DAME

415. MICROSTRUCTURAL EFFECTS IN ABRASIVE WEAR

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

$ 90,000 01-5

Assessment of mechanisms controlling abrasive wear in multiphase alloys, including cast iron; influence of abrasive hardness and angularity; role of wear debris; in-situ SEM scratch tests; change in near-surface microstructure under abrasive wear conditions.

OHIO STATE UNIVERSITY

416. INVESTIGATIONS OF ULTRASONIC WAVE INTERACTIONS AT BOUNDARIES SEPARATING ANISOTROPIC MEDIA

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

$ 90,000 01-5

Research into the interaction of ultrasonic waves with boundaries separating anisotropic materials. Single crystals and bicrystals of nickel are prepared for ultrasonic measurements. Measurements are made of the partitioning of wave energy at an anisotropic-anisotropic boundary and analytical treatment of wave propagation at anisotropic boundaries is included.

417. 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
D. D. Macdonald - Dept. of Metallurgical Engineering
Phone: (614)-422-6255

$ 85,470 (15 months) 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 and distribution; measurement of electrochemical parameters in static and flowing aqueous solutions containing chloride and sulphate ions.

OHIO STATE UNIVERSITY (continued)

418. FUNDAMENTAL STUDIES OF HIGH TEMPERATURE CORROSION REACTIONS

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

$ 88,000 01-1

In-situ SEM study of oxidation of metals, Fe, Ni, Cu and Cr; 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.

419. HYDROGEN ATTACK OF PRESSURE VESSEL STEELS

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

$ 66,107 01-2

The mechanisms which determine the rate of hydrogen attack of pressure vessel steel are studied through a combination of growth kinetic measurements (dilalometry) and careful metallorgraphy. The origin of bubble nuclei is given particular emphasis. In this connection the relative rates of attack in thick section welds and the role of fine weld porosity is given emphasis. The role of matrix creep restraint in limiting hydrogen attack kinetics is studied.

OREGON STATE UNIVERSITY

420. INVESTIGATION OF THE ELECTRICAL AND OPTICAL PROPERTIES OF ORGANOMETALLIC VAPOR PHASE EPITAXIAL $Ga_{1-x}Al_xAs$ AND $Ga_{1-x}Al_xAs$/GaAs INTERFACES IN SOLAR CELLS

P. K. Bhattacharya - Dept. of Electrical and Computer Engineering
Phone: (503)-754-3617

$ 69,098 01-3

Electrical and optical characterization of undoped and intentionally doped $Ga_{1-x}Al_xAs$ layers and $Ga_{1-x}Al_xAs$/GaAs interfaces grown by organometallic vapor phase epitaxial (OMVPE) growth. Measurements extend over the entire mixed alloy composition range of the ternary alloy with particular emphasis on the indirect bandgap region ($x \geq 0.43$) being used for concentrator heterostructure solar cells. Electrical characterization includes detailed study of deep trapping centers in bulk layers and interface regions and transport properties in these regions as a function of alloy composition and temperature. Optical studies include characteristics of the deep states and luminescence measurements. Measurement techniques are Deep Level Transient Spectroscopy, Double Source Differentiated Photocapacitance, capitance-voltage, Hall-effect, velocity-field, and photoluminescence.

PENNSYLVANIA STATE UNIVERSITY

421. HEAT TRANSFER, FLUID FLOW AND ELEMENT VAPORIZATION IN LASER WELDING

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

$ 51,400 01-5

Modelling of solute loss during laser welding of steels based on solution thermodynamics and kinetics data; calculation of local cooling rate and temperature profile, weld pool velocity and propensity for grain growth; correlative experimental determination of weld microstructure and chemistry; measurement of hardness across the weld.

422. CRYSTAL CHEMISTRY OF PORTLAND CEMENT HYDRATES AS RADIOACTIVE WASTE HOSTS

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

$ 50,003 01-1

Detailed study of the crystal chemistry of various hydrated cement phases. Identification of possible crystal chemical substitutions for radioactive waste ions in the crystal structures of the various cement hydrates. Evaluation of the stabilities of substituted cement hydrates. Assemblage of a library of crystal chemical data to be used to optimize cement compositions for use in radioactive waste management.

423. STRUCTURAL PROPERTIES OF AMORPHOUS METALS BY RAMAN SCATTERING

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

$ 78,892 01-1

This study involves the preparation of thin films of amorphous metal alloys by sputtering methods. The optical constants of these films are employed to fabricate trilayer structures for the study of Raman scattering. The materials to be considered initially are iron-boron and iron-phosphorus alloys. The goal of the study is to obtain information on the structure, bonding and thermal stability as a function of temperature, alloy concentration and sputter deposition conditions. The work involves the study of both amorphous and crystalline metal alloys using trilayer Raman scattering.

PENNSYLVANIA STATE UNIVERSITY (continued)

424. MECHANISMS OF WEAR IN SINGLE AND TWO PHASE MATERIALS

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

$ 60,900 (19 months) 01-5

Experimental investigation of two body wear in metals (Al, Cu) and ceramics (Al_2O_3, MgO); effect of contact zone, strain rate and deformation/fracture characteristics of materials.

425. LASER PROCESSING OF CERAMICS

G. L. Messing - Dept. of Materials Science and Engineering
Phone: (814)-865-2262

$ 97,000 (18 months) 01-5

Studies of single component, multicomponent, and decomposition-reaction laser-particle interactions in fine-particle ceramics. Use of a 10.6 micron CO_2 laser to effect calcination without aggregation, morphological modification of particles, and comminution. Thermodynamic and kinetic assessment of effects of rapid heating on processes in fine-particle ceramics, with concerns for potential melting, metamictization, vaporization, and microcracking phenomena. Initial studies will be on Al_2O_3 and MgO particles and their precursors.

426. HYDROGEN ABSORPTION IN METALS: A FIELD ION MICROSCOPY STUDY

H. W. Pickering - Dept. of Materials Sciences and Engineering
Phone: (814)-863-2640

$ 54,000 01-1

Field ion microscopy study of H_2 trapping and absorption in Fe; surface and grain boundary segregation of P and Ti in Ni and H in Fe; quantitative measure of the concentration gradients away from boundaries; cosegregation and clustering of impurities; relationship of above to embrittlement of alloys.

PENNSYLVANIA STATE UNIVERSITY (continued)

427. GRAIN BOUNDARY DIFFUSION AND GRAIN BOUNDARY CHEMISTRY OF CR-DOPED MAGNESIUM OXIDE

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

$ 52,500 01-3

Aliovalent impurity diffusion in ionic materials, specifically Cr in MgO; binding energy between impurities and vacancies; grain boundary diffusion, including diffusion parallel and perpendicular to tilt boundaries; surface diffusion; techniques used--autoradiography, electron microprobe, ion beam spectrochemical analysis.

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

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

$ 60,000 02-2

To study in atomic detail the field adsorption of noble gases and classical molecular gases using the imaging atom probe field ion microscope. Measure the 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.

429. STRUCTURE OF GLASSES CONTAINING TRANSITION METAL IONS

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

$110,000 01-1

Structure and behavior of (1) insulator glasses: silicates, borates, germanates, and phosphates, and (2) modified insulator glasses containing transition metal ions. Leaching and dissolution behavior of glasses. Host glass structure is determined by infrared and Raman spectroscopy. Observed vibrational spectra are related to structural units that make up the glass by means of normal coordinate and other theoretical calculations. Characterization of nearest neighbor environments of transitional metal ions in glasses are carried out by optical absorption spectra, luminescence spectra, and vibrational bands.

UNIVERSITY OF PENNSYLVANIA

430. HIGH CONDUCTIVITY PROTON SOLID ELECTROLYTES

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

$ 94,178 03-1

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

431. MECHANISMS OF DAMAGE ACCUMULATION IN TIME DEPENDENT CYCLIC DEFORMATION

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

$ 63,500 01-2

Identification of microstructural changes resulting from creep and fatigue deformation of metals, initially Cu and low alloy steels; correlation of substructure development with strain hardening and softening during prior monotonic, interrupted or reversed stress cycles; strain burst and relationship to substructure instability; effect of carbide distribution in bainitic steels on strength and transition from trans- to intergranular failure mode; extension of Coffin-Manson low cycle fatigue relation to cyclic creep.

432. INTRINSIC SURFACE PHONONS ON RECONSTRUCTED SEMICONDUCTOR SURFACES

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

$ 78,715 02-3

Theoretical study of the lattice dynamics of reconstructed semiconductor surfaces. Relation between localized surface electronic properties and surface structural and vibrational properties. Computational scheme combines a short range elastic Hamiltonian with a static electronic polarizability extracted from a tight binding representation of the valence electronic bands.

UNIVERSITY OF PENNSYLVANIA (continued)

433. ATOMISTIC STUDIES OF GRAIN BOUNDARIES WITH SEGREGATED IMPURITIES

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

$ 75,000 01-1

Atomistic-based computer simulation of grain boundary structure in dilute and concentrated binary metal alloys, initially Au-Ag, Cu-Ag, and Cu-Bi; development of semi-empirical interatomic potentials incorporating charge transfer and atomic volume and fitted to satisfy lattice parameter and cohesive energy requirements; influence of degree of segregation and boundary periodicity; computation of stress fields around impurities at grain boundaries, and effect of this on co-segregation and H_2 trapping at boundary; structural transitions at boundaries and influence on defect absorption or emission.

434. ELECTROCHEMICAL INVESTIGATIONS OF NOVEL ELECTRODE MATERIALS

W. L. Worrell - Dept. of Materials Science and Engineering
Phone: (215)-898-8592

$ 60,000 03-2

Intercalation of Li, Na and Ca into TiS_2 to form $Li_xNa_yTiS_2$ and $Li_xCa_yTiS_2$, resulting in increased electrical capacity of cathode materials for advanced batteries. Electrochemical studies of electrode performance, and X-ray structural determination of intercalated compounds. Measurement of diffusion coefficient of Li ions; studies of effect of ionic size and charge on stability of intercalant in the TiS_2 lattice. Structural and phase analysis studies will be completed and an isothermal section of the Li-Na-TiS_2 pseudoternary phase diagram will be constructed. Effect of transition metals on Li-Li interaction energy in $Ti_{1-y}Ta_yS_2$ and $Ti_{1-y}Zr_yS_2$.

UNIVERSITY OF PITTSBURGH

435. 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_3) in oxidizing, sulfidizing, and reducing environments; thermogravimetric measurement of corrosion kinetics.

PRINCETON UNIVERSITY

436. STUDIES OF THE DYNAMICS OF MOLECULAR ORIENTATION AND RELAXATION IN POLYMERS BY MEANS OF A MODULATED INFRARED LINEAR DICHROISM TECHNIQUE

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

$ 72,724 03-1

Examine the fundamental relationship between chain conformational changes and resultant macroscopic material responses during deformation. Coupling of rheological and rheo-optical measurements during weld characterized deformation in order to follow the details of molecular orientation and conformational changes.

PURDUE UNIVERSITY

437. NOVEL POLYMERIC Li^+ AND Cd^{2+} FAST ION CONDUCTING MATERIALS; LiI-IODIDE IONENE POLYMERS AND CdI_2-$Cd(PO_3)_2/Cd(PS_3)_2$ GLASSES

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

$ 52,201 01-1

Preparation of plastic fast ion conductors via the formation of a "molten salt" system by dissolution of lithium salts, especially LiI, in iodides of quaternary nitrogen polymeric cations (ionenes). The resulting materials are likely to exhibit high Li^+-ion conductivities, while the polymeric skeleton offers a large range of options for modifying mechanical properties. Investigation of related systems of LiI with monomeric NR_4I salts. Examination of the possibility of obtaining glasses with a relatively high conductivity in which the charge carrier is a divalent cation. The target system is CdI_2-$Cd(PO_3)_2/Cd(PS_3)_2$. Characterizations include electrical conductivity, IR spectroscopy, internal friction and glass transition characterization.

PURDUE UNIVERSITY (continued)

438. ZERO-FLUX PLANES AND FLUX REVERSALS IN MULTICOMPONENT SYSTEMS

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

$ 89,829 01-3

Interdiffusion fluxes of all components in an n-component system are calculated directly from the concentration profiles of a single diffusion couple at any section without invoking Fick's Law or the need for prior knowledge of $(n-1)^2$ interdiffusion coefficients. These studies have identified "zero-flux planes" (ZFP) for individual components, which are planes where the interdiffusion flux of a given component is zero and exhibits reversal in its flow direction on either side of the plane. Objectives include characterization of the ZFP compositions in terms of diffusion paths and thermodynamic data for multicomponent systems.

439. FORMATION OF A PARTICIPATING RESEARCH TEAM AND THE INSTRUMENTATION FOR X-RAY DIFFRACTION AT THE NATIONAL SYNCHROTRON LIGHT SOURCE (Several Institutions Involved)

G. L. Liedl - School of Materials Engineering
Phone: (317)-749-2601

$440,000 01-1

Development of an instrumented beam line and port at NSLS for conducting X-ray crystallography/diffuse scattering experiments on a variety of materials: composites, dilute metal alloys, non-stoichiometric oxides, intermetallic compounds; phenomena of interest--phase transformations, clustering, plastic deformation at crack tips; surface reactions and catalysis; overlayer structure, disordering, and melting; phonon mode softening in phase transitions.

PURDUE UNIVERSITY (continued)

440. MULTICOMPONENT DIFFUSION UNDER GENERAL CHEMICAL POTENTIAL GRADIENTS

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

$ 85,884 01-3

Application of the pair approximation of the Path Probability Method (PPM) of time dependent cooperative phenomena to analytically derive the kinetic matrix of Onsager equations from thermodynamic potentials and some fundamental kinetic parameters such as jump frequencies of component atoms during multicomponent diffusion. Relations among measurable quantities and experimental concepts such as diffusion paths and zero-flux planes in multicomponent diffusion experiments and specific diffusion controlled phenomena in oxides are being investigated.

441. MECHANISMS OF ELEVATED TEMPERATURE RUPTURE IN SINGLE PHASE CERAMICS

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

$ 92,000 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 (1) tensile creep using constant true stress, (2) internal pressurization of pores with inert insoluble gas and microscopic measurement of pore or cavity growth under known hydrostatic pressure and surface tension driving forces. Results are correlated with quantitative microstructural studies of porosity evolution. Materials under investigation are CoO, UO_2, NiO and carbonyl Ni.

RENSSELAER POLYTECHNIC INSTITUTE

442. EXPERIMENTAL TESTS TO UNIFY SINTERING THEORY

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

$ 83,000 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.

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

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

$125,865 02-2

Develop and exploit photon scattering and interaction techniques to study fundamental and applied problems associated with corrosion and catalysis at the solid-liquid interface. Apply surface enhanced Raman scattering. Underpotential adsorption of metal monolayers on metallic substrates. Corrosion chemistry and corrosion inhibition on copper and copper alloys.

444. MOLTEN CARBONATES: MICROWAVE STUDIES OF THE VAPOR STATE

C. W. Gillies - Dept. of Chemistry
Phone: (518)-266-8453

$ 89,034 (18 months) 03-3

Characterization of the vapor state composition of lithium, sodium and potassium carbonates in the temperature range of 650-700^{o}C by microwave spectroscopic studies. Evaluation of optimum operating parameters and electrolyte compositions in fuel cells.

RENSSELAER POLYTECHNIC INSTITUTE (continued)

445. PROTECTIVE OXIDE FILMS

R. K. MacCrone - Dept. of Materials Engineering
Phone: (518)-266-6047
S. R. Shatynski - Dept. of Materials Engineering
Phone: (518)-266-6126

$ 82,000 01-3

Study of both point defects, impurities, and grain boundaries in films of the metal oxides NiO, WO_3, and TiO_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.

446. LOCALIZED CORROSION AND STRESS CORROSION CRACKING BEHAVIOR OF STAINLESS STEEL WELDMENTS

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

$128,000 01-1

Corrosion of ferritic stainless steel weldments and the effect of welding parameters; chloride environments; 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.

RICE UNIVERSITY

447. A STUDY OF THE KINETICS AND THERMODYNAMICS OF HYDROGEN IN Pd-BASED ALLOYS

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

$ 50,175 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. Theoretical investigation of low temperature effects and for H diffusion in Fe. Magnetic susceptibility and elastic constant measurements for Pd and Pd alloys. Statistical thermodynamic modelling.

448. ELECTRON SPIN POLARIZATION EFFECTS IN LOW ENERGY ELECTRON DIFFRACTION, 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

$179,724 02-2

Will use PLEED (polarized LEED) to study surfaces; 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

449. FRACTURE TOUGHNESS PROCESSES

S. J. Burns - Dept. of Mechanical and Aerospace Sciences
Phone: (716)-275-4082

$ 80,000 01-2

Studies of macro-tip dislocation plasticity and the production of microcracks. Materials under investigation include aluminum alloys, various steels, silicon and a number of oxide ceramics. Types of measurements include (a) dislocation nucleation and structures at the tips of cracks, (b) the relationship between positions of dislocations relative to crack-tips and the stress intensity factor for crack propagation, and (c) transmission electron microscopy of dislocations at crack tips.

450. DIFFUSIONAL CREEP OF MULTICOMPONENT SYSTEMS

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

$106,764 01-2

Stress-motivated diffusion; elastic and plastic deformation in ceramic, polymer, and metallic materials; techniques - "impression" creep, fatigue, load relaxation, and elastic deformation; relationships between bulk and impression test data; polycrystals and single crystals; laser excited solid-state reactions, plasticity, and diffusion; Al, β-tin, LiF, KCl, Nb.

ROCKWELL INTERNATIONAL SCIENCE CENTER

451. SINTERING PHENOMENA OF NON-OXIDE SILICON COMPOUNDS

F. F. Lange, T. M. Shaw, P. E. D. Morgan
Phone: (805)-498-4545

$194,982 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

452. METAL ATOM DIFFUSION IN AMORPHOUS SILICA AND AT THE SILICA SURFACE

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

$ 67,000 01-3

Bulk and surface diffusion studies in amorphous silica with the objective of understanding the effects of local structure, interatomic forces, and atom size. Molecular dynamics computer simulation studies in conjunction with EXAFS and SAXS experiments using metal species in bulk amorphous silica. Molecular dynamics computer studies of adatom species in bulk amorphous silica. Molecular dynamics computer studies of adatom species Pd, Pt, or Ag on amorphous silica surfaces to determine the effects of local structure. Specimen preparation by sol-gel processes.

453. HIGH PRESSURE ELECTRON RESONANCE STUDIES OF ELECTRONIC, MAGNETIC AND STRUCTURAL PHASE TRANSITIONS

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

$122,000 02-2

Develop high pressure diamond anvil cell in which to make electron paramagnetic resonance measurements. Use this apparatus to study phase transitions in phosphorus doped silicon, organic charge transfer salts, europium compounds and cesium.

UNIVERSITY OF SOUTHERN CALIFORNIA

454. LIMITING PROCESSES IN LASER CVD

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

$126,468 01-5

Experimental and theoretical research with the objective of developing an understanding of the laser chemical vapor deposition (LCVD) process sufficient to predict deposition rates, microstructures, and resulting film properties. Predictions will account for the effects of surface temperature, laser spot size, local vapor composition, total pressure, optical absorption, thermal properties and thermal expansion mismatch. These variables are to be isolated by means of experiments designed to measure chemical, optical, thermal and mechanical effects. Calculations and measurements of surface temperature and theoretical analysis of convective and diffusive transport correlated with experimental results. Model system: SiC deposited by two types of reactions on various substrates will be investigated to study chemical and transport effects. LCVD of SiC on Mo coated SiC substrate will be used to investigate the effect of changes in optical properties during LCVD. Changes in both optical and thermal properties during LCVD studied by depositing SiC on Mo substrates. Residual interface stresses and their role in LCVD film adherence investigated by depositing SiC on W substrates. Characterization of film thickness profiles, microstructures and film adherence.

455. ELECTRICAL AND MECHANICAL PROPERTIES OF OXIDE CERAMICS

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

$132,000 (17 ½ months) 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)

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

T. G. Langdon - Dept. of Materials Science and Mechanical Engineering
Phone: (213)-741-2095

$125,000 01-2

Measurement of creep and grain boundary sliding in metals; boundary sliding, stress and temperature dependences, threshold creep stress in precipitation hardened and solid solution strengthened Al-base alloys; boundary migration under monotonic as well as cyclic creep; cavitation in Cu alloys and Pb.

SOUTHERN ILLINOIS UNIVERSITY

457. METALLIC GLASSES AND NON-EQUILIBRIUM PHASES AS NEW CATALYSTS IN ENERGY CONVERSION SYSTEMS

W. E. Brower, Jr. - Dept. of Engineering Mechanics and Materials
Phone: (618)-536-2368
G. Smith- Dept. of Chemistry and Biochemistry
Phone: (618)-453-5721

$ 77,000 01-1

Identification of the catalytic activity of non-equilibrium crystalline and amorphous metals, specifically Pd- and Ni-base alloys, and the role of defects thereon; characterization of microstructure and transformation kinetics of rapidly-cooled alloys; use of molecular probe.

SOUTHWEST RESEARCH INSTITUTE

458. THE STUDY AND MODELLING OF HIGH TEMPERATURE FATIGUE CRACK PROPAGATION IN AUSTENITIC STAINLESS STEEL

D. L. Davidson - Dept. of Materials Sciences
Phone: (512)-684-5111

$ 45,000 01-2

In-situ observation of crack tip strain fields in austenitic stainless steels under creep and creep-fatigue loading, and correlation with microstructural features; techniques used: SEM, electron channeling, and optical stereo imaging.

SOUTHWEST RESEARCH INSTITUTE (continued)

459. CHARACTERIZATION AND ANALYSIS OF CAVITY DEVELOPMENT DURING CREEP OF CERAMICS AT ELEVATED TEMPERATURES

R. A. Page - Dept. of Materials Science
Phone: (515)-684-5111, x3252
J. Lankford - Dept. of Materials Sciences
Phone: (515)-684-5111, x2317

$ 80,148 01-2

Determination of cavity nucleation and growth rates as a function of (incubation) time, applied compressive stress, and microstructure during the early stages of creep in Al_2O_3 and SiC. Cavitation creep modelling. This experimental research is based on the use of the 30m SANS (small angle neutron scattering) instrument at ORNL with measurements to be performed over the angular range $5x10^{-3}$ Å$^{-1} \leq q \leq 3.5x10^{-2}$ Å^{-1} with neutrons of wavelength 4.75Å and an angular resolution of approximately $1x10^{-3}$ Å^{-1}. SANS data will be reduced to yield the radius of gyration, Porod radius total cavity surface area, total cavity volume, and total cavity number. Density measurements by a sink-float technique on a specimen suspended within a temperature-controlled pyncnometer. Dark field and lattice fringe imaging electron microscopy.

STANFORD UNIVERSITY

460. PHOTOELECTRONIC PROPERTIES OF II-VI HETEROJUNCTIONS

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

$187,094 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.

STANFORD UNIVERSITY (continued)

461. EVALUATION OF MACHINING DAMAGE IN BRITTLE MATERIALS

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

$102,600 01-5

NDE measurement of cracks and residual stress induced by machining ceramics, initially Si_3N_4, and a model brittle material, Si; crack size determination with acoustic and laser techniques, and residual stress level with acoustic methods.

462. MODELLING OF DEFORMATION AND FRACTURE IN HIGH-TEMPERATURE STRUCTURAL MATERIALS

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

$172,200 01-2

Development of quantitative methods of predicting deformation and fracture of metals and alloys subjected to complex histories and environments; computer based constitutive equations for non-elastic deformation, "MATMOD"; modelling of fatigue crack initiation and growth, "FATIGMOD"; modelling of multiaxial plastic flow; applications to Type 304 stainless steel, 2 1/4 Cr-1 Mo steel and Al alloys.

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

D. V. Nelson - Dept. of Mechanical Engineering
Phone: (415)-497-2123
J. C. Shyne - Dept. of Materials Science and Engineering
Phone: (415)-497-2535

$124,300 01-5

Investigation of fatigue crack growth in austenitic stainless and martensitic low alloy steels, using surface acoustic waves as a probe of crack depth and closure stress; influence of crack tip plasticity on acoustic method; correlation of crack propagation rate, crack closure stress, and cyclic stress ratio.

STANFORD UNIVERSITY (continued)

464. A STUDY OF THE MICROSTRUCTURAL PROCESSES WHICH CONTROL HIGH TEMPERATURE CRACK GROWTH

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

$ 80,397 01-2

Study of creep deformation, cavitation, and cracking in metals (Cu and Ni) with either impurity segregation or with an array of gas bubbles at grain boundaries; stress field at creep crack tips; correlation of crack growth with grain size, degree of segregation, and creep deformation parameters; identification of mechanisms controlling creep crack growth.

STEVENS INSTITUTE OF TECHNOLOGY

465. 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

$ 84,000 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

466. THE CATALYTIC REACTIVITY OF CRYSTAL SURFACES

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

$119,000 01-1

Characterization of topography of thin single crystal metal films (Pd, Pt); measurement of the adsorption kinetics of O_2, CO, and hydrocarbons on these films; identification of film growth mechanism; correlation of film defect structure with adsorption behavior; relation of above to catalytic activity; techniques used - LEED, AES, EELS.

UNIVERSITY OF TEXAS

467. POLAR FLUIDS: PHOTOEMISSION AND ELECTRONIC ENERGY LEVELS

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

$ 90,009 02-2

Measure photoinjected current in polar fluids (NH_3, H_2O and alcohols) as a function of bias, photon energy and temperature. Ag electrode illuminated by pulsed dye laser. Measure i-V curves and determine electronic energy levels, interfacial work functions. Concurrent theoretical work includes calculation of density of states.

UNIVERSITY OF UTAH

468. MULTI-SPECTROSCOPIC STUDIES OF THE ELECTRONIC STRUCTURE OF ELECTRODE MATERIALS FOR HIGH ENERGY DENSITY BATTERIES: I-II AND I-III INTERMETALLIC COMPOUNDS WITH B32 STRUCTURE

I. M. Curelaru - Dept. of Materials Science and Engineering
Phone: (801)-581-3589

$ 75,000 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 non-stoichiometry, 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 data with existing LCAO, cluster model, and self-consistent linear muffin-tin LMT band-structure calculations.

UNIVERSITY OF UTAH (continued)

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

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

$ 66,426 01-3

Miscibility gap studies in III-V quaternary alloys, including (1) development of models and techniques for calculating solid-solid miscibility gaps in quaternary alloys, (2) calculation of effects of coherency strain on the equilibrium phase diagram, (3) experimental determination of the miscibility gap in the system $Ga_xAl_{1-x}As_{1-y}Sb_y$ in both homogeneously nucleated platelets (without elastic strain) and liquid phase epitaxial layers on GaAs and InP substrates, (4) calculating the effects of elastic strain in epitaxial growth, and (5) miscibility study of $Ga_xAl_{1-x}As_{1-y}Sb_y$ alloys grown by the kinetically controlled organometallic vapor phase epitaxial technique. Investigation for nonequilibrium alloys of spinodal decomposition and its effects on the electrical and optical properties of the alloys. STEM and X-ray analysis.

VIRGINIA POLYTECHNIC INSTITUTE AND STATE UNIVERSITY

470. FRACTURE MECHANISMS IN GLASS-CRYSTAL COMPOSITES

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

$ 99,392 (17 months) 01-2

Fracture mechanisms in glass-crystal composites with a cordierite glass-ceramic and its original (non-crystallized) glass 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 or 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.

VIRGINIA POLYTECHNIC INSTITUTE AND STATE UNIVERSITY (continued)

471. HYDROGEN EMBRITTLEMENT TESTING

M. R. Louthan, Jr. - Dept. of Materials Engineering
Phone: (703)-961-6640

$ 25,000 01-2

Evaluation of the effective H_2 fugacity in electrochemically-charged steels by comparison with gaseous permeation data; mechanical testing of carbon and low alloy steels either electrochemically charged or in gaseous hydrogen up to 65 MPa; effect of chemical poisons on H_2 ingress; influence of pre-existing flaws on susceptibility to embrittlement.

UNIVERSITY OF VIRGINIA

472. SPECTROSCOPY OF SURFACE ADSORBED MOLECULES
R. V. Coleman - Dept. of Physics
Phone: (804)-924-3781

$ 96,000 02-2

Investigations of the properties of surfaces and interfaces containing molecular adsorbates using inelastic electron tunneling (IETS), photoemission (ESCA), and Auger spectroscopies. IETS spectra will be obtained for a number 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 will be made on the same systems to augment the IETS work. Studies of UV-induced damage to molecules and photocatalytic effects on semiconductor oxides.

473. MAGNETIC IMPURITIES IN SUPERCONDUCTORS

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

$ 80,057 02-3

Theoretical research on magnetic impurity interactions in superconductors. Study of rare earth impurities in various metallic hosts to determine relative importance of exchange interactions and to examine electronic structural basis for coupling. Studies on influence of impurities, at intermediate concentrations, on the electron spin susceptibility and nuclear spin relaxation rate. Continuing emphasis on investigating new mechanisms for achieving enhancement of superconducting properties in high magnetic fields.

UNIVERISTY OF VIRGINIA (continued)

474. THE EFFECT OF MICROSTRUCTURE ON THE FATIGUE BEHAVIOR OF Fe-C-X ALLOYS

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

$ 60,500 (15 months) 01-2

Experimental correlation of fatigue behavior of duplex martensitic-ferritic steels with microstructural features such as carbide type, morphology and distribution, and continuity of ferrite vs. martensite; crack initiation and propagation in high and low cycle fatigue; crack cloture effects.

UNIVERSITY OF WASHINGTON

475. NUCLEAR MAGNETIC RESONANCE STUDIES OF ION MOTION IN SOLID ELECTROLYTES

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

$ 89,205 01-3

Nuclear magnetic resonance (NMR) studies of spin-spin and spin-lattice relaxation times, effects of motion and structure upon the electric quadrupole NMR spectrum, and direct NMR diffusion measurements to study the solid electrolytes mixed cation β-alumina, phosphoborate glasses, and lithium iodide monohydrate. Correlative studies involve electrical conductivity and thermal analysis. Temperature and frequency dependence of the spin-lattice relaxation to understand ion-ion and ion-lattice interactions and predict electrolyte systems with optimized conductivity. Other techniques invoked include thermogravimetric analysis, X-ray diffraction, infrared absorption, thermomodulated uv-reflectivity and thermoelectric currents.

476. RUBBER ELASTICITY

B. E. Eichinger - Dept. of Chemistry
Phone: (206)-543-1653

$ 151,270 (24 months) 03-1

Experimental studies of the elastic contribution to the chemical potential of a swelling agent in crosslinked and uncrosslinked polydimethlsiloxane. Theoretical studies on eigenvalue spectra of Kirchoff matrices which describe random networks. Characterization using small angle X-ray scattering.

UNIVERSITY OF WASHINGTON (continued)

477. X-RAY SPECTROSCOPY OF SOLIDS UNDER PRESSURE

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

$ 70,000 02-2

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

UNIVERSITY OF WEST VIRGINIA

478. ELECTRON HYBRIDIZATION EFFECTS AND THE CRYSTAL STRUCTURE OF PLUTONIUM

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

$ 56,953 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/MILWAUKEE

479. MICROSTRUCTURAL ANALYSIS OF ION-CONTAINING POLYMERS

S. L. Cooper - Dept. of Chemical Engineering
Phone: (608)-262-3641

$ 82,820 03-1

Studies of microstructure of several ionomer systems by SAXS, EXAFS and Mössbauer spectroscopy. Characterization of size and separation of ionic domains using correlation function derived from small angle X-ray scattering measurements. Investigations of relationships between composition and preparation variables and morphology and transport properties.

UNIVERSITY OF WISCONSIN/MILWAUKEE (continued)

480. INTERACTION OF LOW ENERGY ELECTRONS WITH SURFACE LATTICE VIBRATIONS

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

$ 74,985 02-2

Theory of electron energy loss spectroscopy (EELS) of 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 D. L. Mills, University of California-Irvine.

UNIVERSITY OF WISCONSIN/MADISON

481. INVESTIGATION OF AMORPHOUS METAL FILMS 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

$ 75,000 01-1

Experimental investigation of the structure, stability, and atomic transport behavior of high-T_g amorphous-metal films on semiconductor substrates. RF sputtering deposition of thin amorphous films of Ni-Nb, Mo-Si, and W-Si alloys on semiconductor substrates of Si, GaAs, and GaP. Characterization of crystallization kinetics, crystallization mechanism, and film/substrate interdiffusion at temperatures near the glass-transition temperature by structural, calorimetric, and electrical measurements. Examination of structural relaxation by electrical resistivity measurements during post-deposition annealing. Measurement of diffusion and interdiffusion by a combination of Rutherford back scattering and Auger electron spectroscopy techniques. Assessment of reactions involving crystallization and possible phase separation, involving TEM analysis of in-situ annealing, and supplementary SEM and X-ray diffraction measurements.

UNIVERSITY OF WISCONSIN/MADISON (continued)

482. OPTICAL STUDIES OF DYNAMICAL PROCESSES IN DISORDERED MATERIALS

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

$ 80,000 (6 months) 02-2

This program is 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 will be developed to be used in conjunction with an existing facility for Fluorescence Line Narrowing. The first component of this program will investigate the temperature dependence of the relation effects in disordered materials and testing of disordered materials will be investigated to determine the microscopic interactions and to extend the models. The third phase will be a fundamental study of ion transfer, trapping, and cross relaxation in a prototypical glass system.

SECTION C

Small Business Innovation Research

This information was prepared by the DOE-Division of Materials Sciences project manager. All projects are Phase I, with the goal to determine, insofar as possible, the scientific or technical merit and the feasibility of ideas submitted under the SBIR program. Phase I funding is limited to less than $50,000 per project for a period generally of less than six months.

ALTEX CORPORATION

500. EXTREME ULTRAVIOLET AND SOFT X-RAY INSTRUMENTATION FOR MICROCHARACTERIZATION OF MATERIALS

H. Pummer
(312)-996-7499

SBIR

The objective of the proposed research program is to quantify the key factors which determine performance, complexity, and cost of an excimer laser system for the generation of coherent high spectral brightness radiation in the extreme ultraviolet and soft x-ray spectral regions. The first phase of this research effort will center on the critical issue of the generation of a high quality picosecond seed beam suitable for amplification in excimer lasers. The efficiency of different frequency conversion schemes and the characteristics of various pulse slicing techniques will be studied. Finally, a feasibility and cost study for a commercial picosecond excimer laser system suitable for short wavelength generation will be performed.

CERAMIC FINISHING COMPANY

501. FRACTURE MECHANICS INVESTIGATION OF GRINDING OF CERAMICS

H. P. Kirchner
(814)-238-4270

SBIR

Application of contact fracture mechanics to investigate mechanisms of material removal and damage penetration during abrasive machining of ceramics. In Phase I it is planned to emphasize investigation of the mechanisms of material removal including crushing by mixed mode fracture ahead of the diamond point and chipping at lateral cracks propagating in response to residual stresses induced by elastic relaxation against the irreversibly deformed zone on unloading. The objective is to 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. The role of crushing in reducing the residual stresses that are responsible for lateral cracking will be investigated. Mathematical models will be developed by adapting available models for static indentations. The experimental results will be compared with results predicted by these models.

CERES CORPORATION

502. HORIZONTAL GROWTH OF SILICON SHEET CRYSTALS VIA EDGE-SUPPORTED PULLING (ESP) FROM A MELT CONTAINED IN A COLD CRUCIBLE

J. F. Wenckus
(617)-899-5522

SBIR

The program will 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. However, the sheet growth rates achieved to date are severely restricted by the rate of heat dissipation from the narrow sheet/melt interface. Moreover, since the filaments in the ESP process pass through holes in the bottom of the melt container, shallow melt levels must be used and melt replenishment during growth has yet to be achieved. This program will endeavor to integrate the unique operational features of the cold crucible with the equally unique attributes of the ESP process in order to demonstrate the feasibility of the horizontal edge-supported pulling (HESP) method for the production of silicon crystals.

ELECTROCHEMICAL TECHNOLOGY CORPORATION

503. MATHEMATICAL MODELING OF STRESS CORROSION CRACKING

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

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.

FIBER MATERIALS, INC.

504. HIGH PERFORMANCE SILICON CARBIDE AND SILICON NITRIDE

H. D. Batha
(207)-282-5911, x280

SBIR

Hot isostatic pressing (HIPing) of silicon nitride and silicon carbide in nitrogen in order to define operating conditions, raw material properties and the role of certain additives required to produce bodies with superior strength and toughness. Investigation of the role of microstructural acicular SiC or Si_3N_4 on strengthening and the formation of ceramic fiber reinforced ceramics.

MEASUREMENT CONCEPTS, INC.

505. DEVELOPMENT OF A SINGLE APERTURE-FOUR CHANNEL NANOSECOND POLARIMETER FOR APPLICATION TO THE NON-DESTRUCTIVE EVALUATION (NDE) OF MATERIALS

E. Collett
(201)-780-7576

SBIR

The design and fabrication of a new type of polarimeter called a Single Aperture-Four Channel Optical Polarimeter will be undertaken. It is designed to measure simultaneously the four Stokes polarization parameters of an optical beam and is capable of measuring the Stokes parameters of either a cw or pulsed optical beam and is readily adapted to ellipsometry. If a dielectric film is illuminated with a single pulse of right or left circularly polarized light then the index of refraction and the thickness of the thin-film can be found non-destructively.

SUPERCON, INC.

506. AN INVESTIGATION TO DETERMINE THE COMMERCIAL FEASIBILITY OF IN SITU Cu-Nb COMPOSITES FOR HIGH STRENGTH, HIGH CONDUCTIVITY APPLICATIONS

J. Wong
(617)-655-0500

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.

TECHNOLOGY FOR ENERGY CORPORATION

507. A HIGH-SPEED, CURVED, POSITION-SENSITIVE X-RAY DETECTOR

R. W. Hendricks
(615)-966-5856, x2524

SBIR

A new high-speed, curved position-sensitive x-ray detector will be developed. The design will circumvent several of the limitations of current linear position-sensitive detectors. The unique features of the proposed detector are: multiple anode wires in a unique spacing arrangement which will distribute the space charge over a wider area and will lead to both longer detector lifetime and higher count-rate capability; and a new concept for a planar fan-shaped cathode wire meander which allows both finer wire spacings and higher resistance and thus high spatial resolution on a curved array.

UNIVERSAL ENERGY SYSTEMS, INC.

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

P. P. Pronko
(513)-426-6900

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; comparison with crystalline metal behavior.

SECTION D

Collaborative Research Centers

Basic materials research which is long range, generic in nature, is conducted by the Office of Basic Energy Sciences/Division of Materials Sciences to provide an underpinning for the development of energy systems. In the pursuit of these research goals, facilities or centers which are unique and/or expensive and costly to reproduce elsewhere have been and are being developed. 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 a number of the most important centers together with a statement of the method of gaining access to them. The collaboration carried out by outside users has 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. In addition, 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, it is recommended that the reader make use of the laboratory contacts 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 pole 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 biologists, chemists, solid state physicists, metallurgists, 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	20Å $< \lambda <$ 2000Å; 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, fluourescence, 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	100 Å $< \lambda <$ 1000 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: $0.03 < Q < 10\ Å^{-1}$
Biology	
Small Angle Neutron Scattering	Studies of large molecules. Located on cold source with $20 \times 20\ cm^2$ position-sensitive area detector. Sample detector distance $L < 2$ meter Incident wavelength $4\ Å < \lambda_o < 10\ Å$
Diffractometer	Protein crystallography $20 \times 20\ cm^2$ area detector $\lambda_o = 1.57\ Å$
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: $0.025\ eV < E_o < 25keV$
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 triple-axis polarized-beam spectrometer, the double-crystal small-angle diffractometer, and the correlation chopper.

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. Travel and living expenses are also the user's responsibility. 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 x 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 x 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 x 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 x 10^{-5} $Å^{-1}$
HB-4A	Four-circle diffractometer	Beam size - 5 x 5 mm Flux - 2 x 10^6 neut/cm^2 sec with 9' collimation λ = 1.015 Å
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 (IPNS-I)

Argonne National Laboratory
Argonne, Illinois 60439

IPNS-I 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 opportunities:

- o high fluxes of epithermal neutrons (0.1-10 eV)
- o pulsed nature, suitable for real-time studies and measurements under extreme environments
- o very low gamma-ray backgrounds

Three principal types of scientific activity are underway at IPNS-I: 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; inelastic neutron scattering, concerned with processes where the neutron exchanges energy and momentum with the system under study and thus probes the dynamics of the system at a microscopic level; and neutron radiation effects, concerned with the defect cascades produced in a material by a fast neutron radiation field and the effect of these cascades on its physical properties. 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 resonance neutron radiography.

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-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

INTENSE PULSED NEUTRON SOURCE (IPNS-I)

TECHNICAL DATA

NEUTRON SCATTERING

Facility (Instrument Scientist)	Assignment	Range †Wave-vector	Range Energy	Resolution Wave-vector	Resolution Energy
Special Environment Powder Diffractometer (J. D. Jorgensen)	F5	0.5-40 $\mathring{A}^{-1}$	*	0.35%	*
General Purpose Powder Diffractometer (J. Faber, Jr.)	F2	0.5-100 $\mathring{A}^{-1}$	*	0.25%	*
Single Crystal Diffractometer (A. J. Schultz)	H1	2-20 $\mathring{A}^{-1}$	*	2%	*
Low-Resolution Medium-Energy Chopper Spectrometer (C.-K. Loong)	F4	0.1-30 $\mathring{A}^{-1}$	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 $\mathring{A}^{-1}$	0-0.4 eV	0.01 K_o	0.02 E_o
Small-Angle Scattering Diffractometer (J. E. Epperson (a), C. Borso (b))	C1	0.001-0.3 $\mathring{A}^{-1}$	*	0.004 $\mathring{A}^{-1}$	*
Crystal Analyzer Spectrometer (T. O. Brun)	F1	3-16 $\mathring{A}^{-1}$	0.02-0.5 eV	3%	2%

* No energy analysis
† Wave-vector, $K = 4\pi \sin\theta/\lambda$
(a) Materials Science -- 3 Meter Flight Path
(b) Biology -- 8 Meter Flight Path

NEUTRON BEAMS AVAILABLE 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

RADIATION EFFECTS

Facility (Instrument Scientist)	Description
Radiation Effects Facility (R. C. Birtcher)	Two vertical (5 cm ID) tubes with flux 1 x 10^{12} n/cm^2 sec and one horizontal (3.8 cm ID) tube with flux 3 x 10^{11} for energy greater than 0.1 MeV at 8μA; capabilities for maintaining two samples at liquid helium temperature (4°K) and above

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 WNR using the advantages of time-of-flight methods. Available instruments include: 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 liquids 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 WNR/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 nonsensitive 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

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(FTS) 843-6069

SNR/PSR

TECHNICAL DATA

	1982	1985
Proton Source	LAMPF	LAMPF + PSR
Proton Source Current	750μA	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)	$1.6 \times 10^{11}/E$	$3.2 \times 10^{12}/E$
Peak Thermal Flux ($n/cm^2.S$)	5×10^{13}	1×10^{16}

User Instrument	Purpose and Description
General Purpose Powder Diffractometer	Liquids and amorphous metals, powder diffraction wave vector 0.3-50Å^{-1} resolution 0.45% powder 2% liquids
Single Crystal Diffractometer	Laue time-of-flight spectrometer wave vector 1-15Å^{-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
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 s^{-1} 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

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 newly installed 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). In late 1983, a 200 kV analytical microscope will be added. Facilities for image simulation, analysis, and interpretation will also be 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. A. Simnad, Chairman; W. L. Bell, J. M. Gibson, D. A. Howitt, J. J. Hren, J. C. H. Spence, and A. Taylor; internal members are G. Thomas, R. M. Glaeser, 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.

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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

-5006

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 (ARM) (available about August 1983)	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 (planned)	X-ray and energy-loss spectrometers micro-diffraction (CEB)	100 kV - 200 kV state-of-the-art resolution

HIGH VOLTAGE ELECTRON MICROSCOPE TANDEM FACILITY

Argonne National Laboratory
Argonne, Illinois 60439

The Argonne National Laboratory High Voltage Electron Microscope-Tandem Facility provides unique combinations of the techniques of high-voltage electron microscopy, ion implantation/bombardment, and ion-beam analysis.

The high-voltage electron microscope is an improved Kratos/AEI-EM7 with a maximum voltage of 1.2 MV, and a demonstrated lattice resolution of 3.5 Å. In addition to a 33° ion-beam access tube, the microscope contains a number of specialized features. These include a negative ion trap, an ion-pumped specimen chamber, two independently adjustable dark-field conditions, a 100-1200 kV continuous-mode voltage selection from the control desk, and a beam dosimetry system for both the ion and the electron beams. A variety of side entry single and double tilt stages are available, which permit observations between 10 and 1000 K in vacuo, and from ambient to 1300 K in gaseous environments. Two straining stages are also available for work either in vacuo or in the environmental cell. The ANL HVEM is equipped with a Harwell design camera, and a Cohu video camera and image intensifer are mounted beneath the microscope column.

A National Electrostatics 2 MV Tandem Ion Accelerator and a 300 KV ion accelerator together can produce ion beams from 10 keV to 8 MeV of most stable elements in the periodic table. The tandem unit has two external negative ion sources and a positive ion source in the terminal. Ions from the accelerators can be transported into the microscope through the "ion-beam interface" to permit direct observation of the effects of ions as well as electron bombardment on materials in the HVEM.

USER MODE

The HVEM-Tandem facility is operated as a national materials science resource. Qualified scientists wishing to conduct experiments should submit a proposal to the person named below. Decisions as to which experiments will be done are made by a Program Advisory Committee following peer evaluation of the proposals. There are no use charges for users carrying out basic research of documented interest to DOE. Use charges will be levied for proprietary investigations.

PERSON TO CONTACT FOR INFORMATION

A. Taylor
Manager, HVEM-Tandem Facility
Argonne National Laboratory
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Argonne, Illinois 60439

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ARGONNE NATIONAL LABORATORY HIGH VOLTAGE ELECTRON MICROSCOPE-TANDEM FACILITY

TECHNICAL DATA

Instrument	Key Features
KRATOS 1.2 MeV Electron Microscope	Resolution 3.5 Å lattice Magnification 63-1,000,000X Continuous voltage selection Current density 15 A/cm^2 High-vacuum specimen chamber Two switched dark field conditions Negative ion trap Electron dosimetry system Cohu video system Ion beam access port Cryogenic anticontaminator
Accelerators	
NEC Model 2 UDHS	Terminal voltage - 2 MV Energy stability - ±250 eV Current density - H^+ 10 μA/cm^2 (typical) Ni^+ 1 Pt^+ 0.1
Texas Nuclear 300-kV	Terminal voltage - 300 kV Energy stability - ±300 eV Current density - H^+ 20 μA/cm^2 (typical) Ni^+ 2 Pt^+ 2
Ion Sources	Available for both accelerators: Danfysik 910, 911 Sputter Duoplasmatron External for tandem: Alphatros SNICS
Ion Beams	Any stable isotope
Beam Lines	Ion-beam interface to HVEM Beamlines and target chambers for irradiation and in beam analysis Dual-ion target chamber

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, and analytical (energy dispersive x-ray spectroscopy and electron energy loss spectroscopy). 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. 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

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SHARED RESEARCH EQUIPMENT PROGRAM (SHaRE)

Technical Data

Instruments and Facilities	Key Feature	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; energy dispersive x-ray analysis; electron energy loss spectroscopy; convergent beam electron diffraction	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; energy dispersive x-ray analysis; electron energy loss spectroscopy	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

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, microcrystallography, surface analysis, etc. A team of professionals runs the facility and its members facilitate the research.

USER MODE

Most of the research in the facility is funded by MRL contracts of the University of Illinois faculty, and is carried out by graduate students, post-doctoral and faculty researchers and by the Center's own professional staff.

For the benefit of external users the system retains as much flexibility as possible. The preferred form of external usage is collaborative research through a contract with a faculty member associated with the MRL, or by direct negotiation with the management of the Center. Direct user access to the equipment is also possible, for trained individuals. In all cases, the research carried out by facility users has to be in the furtherance of DOE objectives.

The facility staff maintain training programs in the use of the equipment and teach associated techniques. An increasing part of the Center's activity is concerned with the development of new instruments and instrumentation.

A brochure describing the Center and its services is available.

PERSON TO CONTACT FOR INFORMATION

Dr. J. A. Eades, Coordinator (217)-333-8396
Center for Microanalysis of Materials
Materials Research Laboratory
University of Illinois
104 S. Goodwin
Urbana, Illinois 61801

CENTER FOR MICROANALYSIS OF MATERIALS

Instruments

Imaging Secondary Ion Microprobe Cameca IMS 3f	Mass analysed images to 0.3μ res. Positive and negative ions.
Scanning Auger Microprobe Physical Electronics 595	Resolution: SEM 300 Å, Auger 700 Å. Windowless X-ray detector.
Scanning Auger Microprobe Physical Electronics 545	Resolution: SEM 3μ. Specimen temp: 77-600 K.
XPS Physical Electronics 548	Double pass CMA. ESCA and Auger analysis. Specimen temp. to 1550 K.
Transmission Electron Microscope Philips EM420 (120kV)	EDS, EELS, STEM. Cold stage (30K). Computer Control.
Transmission Electron Microscope Philips EM400T (120kV)	EDS. Heating, cooling stages.
Scanning Transmission Electron Microscope Vacuum Generators HB 5 (35kV)	5Å probe, EDX, EELS.
Scanning Electron MIcroscope JEOL JSM 35C (35kV)	50Å resolution, EDX.
Rutherford Backscattering (in-house construction) (3 MeV)	Under development
X-ray Equipment Elliott 14 kW high brilliance source Rigaku 12 kW source Several Conventional Sources	4-circle diffractometer. Small angle camera. EXAFS. Lang topography. Powder cameras, etc.
Transmission Electron Microscope (300 kV)	Delivery winter 1983/1984

In addition to the main items listed above the Center also has other equipment: a second scanning electron microscope, two electron microprobes, 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, an acid saw, etc.

The equipment is made available on a flexible week-by-week booking scheme; if professional help is required, operating hours at 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

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Oak Ridge National Laboratory
Post Office Box X
Oak Ridge, Tennessee 37830

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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.
10–200-KV High-Current Ion Implantation Accelerator	Essentially any species of ion. 1–10 mamps singly charged, ∿100 μamps doubly and triply charged.
0.1–10-KeV Ion Gun	Gaseous species. ∿100 μamp.
Lasers	
Pulsed Ruby Laser (0.6943 μm)	15–30 x 10^{-9} s pulse duration time. 10 Joule/Pulse Output Multimode, 2-1/2 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 Nd:YAG/Glass Laser Wavelengths: 1.06 μm, 0.530 μm, 0.353 μm, 0.265 μm	15 x 10^{-9} s. 20 Joule/Pulse (1.06 μm), 5 Joule/Pulse (0.530 μm), 1 Joule/Pulse (0.265 μm). 30,50,100 or 200 x 10^{-12} s. 0.7 Joule/Pulse (1.06 μm) 0.2 Joule/Pulse (0.530 μm), 0.07 Joule/Pulse (0.265 μm).
Pulsed Excimer Laser (0.308 μm)	20 x 10^{-9} s. 1.5 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. Optical emissions from sputtered particles. 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 diagnostics, primarily spontaneous Raman spectroscopy, are being developed and used to study high temperature corrosion and erosion of materials for combustion systems. Emphasis is on the use of these techniques to identify chemical compounds present on surfaces during attack in hostile environments. In-situ analyses can be obtained with excellent temporal resolution (approximately 10 spectra per second) from samples in high temperature corrosive environments. Both pulsed and continuous lasers at various wavelengths throughout the visible and ultraviolet are available for excitation of Raman scattering, which can be detected using photon counting, gated integration, or optical multichannel techniques. These measurements are complemented by post-exposure Raman measurements including a Raman microprobe which allows analysis with micron spatial resolution. Other techniques including Sputter Induced Photon Spectroscopy (SIPS), Scanning Auger Microscopy (SAM), X-ray diffraction, and metallographic analysis provide complementary compositional and morphological information. Present research concerns include oxidation-sulfidation of Fe-Cr and Fe-Mn-Al alloys, chemical attack of stabilized zirconia thermal barrier coatings, corrosion of ion-implanted metals, and combined oxidation-erosion of steel. The goal is to obtain information about attack mechanisms utilizing data obtained during the corrosion processes.

Equipment which is available in a collaborative mode also includes the atmospheric combustor exhaust simulator (ACES) which produces an environment for realistic corrosion/erosion studies with capability for in-situ Raman analysis. ACES provides a high velocity (50 feet per second), high temperature (1000°C) gas flow with provision for particulate injection. This apparatus is being used for in-situ Raman studies and for erosion experiments.

USER MODE

This materials program at Sandia has emphasized research into corrosion and erosion mechanisms using the techniques and equipment described above. Interactions include collaborative research projects with outside users and providing information on new diagnostic approaches to the study of corrosion. In initiating collaborative research projects it is generally desirable to perform preliminary Raman analyses of typical samples and of reference materials to determine sensitivity to expected corrosion products. Subsequently, 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 labs 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 8342
Sandia National Laboratories
Livermore, California 94550

(415)422-3126
FTS 532-3126

COMBUSTION RESEARCH FACILITY - MATERIALS PROGRAM

TECHNICAL DATA

Instruments	Key Features
Raman Spectrometer	Rejects elastic light to within 50 cm^{-1} of laser line.
	100 ms. temporal resolution.
Raman Microprobe	1 micron spatial resolution.
Sputter Induced Photon Spectroscopy (SIPS)	5 keV argon beam surface analysis of insulators.
Atmospheric Combustor Exhaust Simulator	50 fps flow 1000°C temperature Particulate 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

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FTS 865-5236

LOS ALAMOS EQUATION OF STATE LIBRARY CENTER*

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

The Los Alamos Equation of State (EOS) Library is a computer-based library of EOS data and FORTRAN subroutines developed at Los Alamos. It is used nationally and internationally by many Laboratories, universities, research institutes and private corporations. The Library is becoming a standard reference resource for EOS and related data.

The Library contains EOS tables of pressure and internal energy as functions of temperature and density for approximately 50 different materials. The tabular format has several advantages: (1) it can represent phase transitions accurately, (2) it covers a wide range of temperatures and densities, and (3) it is easily updated to incorporate new experimental or theoretical results in specific regions of temperature and density. All types of materials are tabulated, including gases, metals, ceramics, plastics, glasses, and even composites such as rocks and minerals.

The associated subroutine library contains programs to update and retrieve data for a given material as well as accurate interpolation schemes for that data. These subroutines can be used directly in the user's computer program and have been incorporated in a number of Lagrangian and Eulerian fluid dynamic codes. The tables are sent from Los Alamos to other institutions on magnetic tapes, in a format that can be interpreted even if the other installation has a computing system different from that at Los Alamos. In most cases, the user can begin to apply the new table to a problem without having to analyze, interpret, or adapt it to his particular needs. Information about the availability of new data is communicated to users by journal articles, reports, informal newsletters, and by personal contact.

The EOS tables usually cover a much wider range of pressure and temperature than can be studied by experimental methds. To construct the tables, it is necessary to employ theoretical models of solids, liquids, vapors, and plasmas, for mixtures and chemical compounds as well as pure elements. EOS tables of high standard from sources other than Los Alamos, even though of more restricted pressure-temperature ranges, are also incorporated in the Library. Other related material properties, such as radiative opacities and conductivities, are available.

USER MODE

The Los Alamos EOS Library is available to users free of charge. To obtain the Los Alamos EOS Library, a user should send a list of materials required and two magnetic tapes with write format specification to

SESAME Library, T-4, MS B212
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

PERSON TO CONTACT FOR INFORMATION

Stanford P. Lyon
MS B212
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

(505) 667-7024
(FTS) 843-7024

LOS ALAMOS EQUATION OF STATE LIBRARY

TECHNICAL DATA

Materials

Air (dry)
Alumina (Al_2O_3)
Aluminum
+ Ammonia
Argon

Beryllium
Boron carbide
Brass
+ Butane (normal)

+ Calcium carbonate
Carbon (liquid)
Carbon phenolic
Copper

Deuterium
+ Deuterium-tritium mixture
+ Deutero-polyethylene
Diamond

Granite (Westerly)
Gold

Helium
High explosive
Hydrogen

Iron

Krypton

Lead
Lithia-boria glass
Lithium
Lithium deuteride
Lithium hydride

Mica
Methane
Molybdenum

Neon
Nevada alluvium
Nickel
Nitrogen
Oxygen

PBX-9502 (explosive)
Platinum
+ Polyethylene (branched)
+ Polyethylene (linear)
Polystyrene
+ Polytetraflouroethylene
Polyurethane

Quartz (SiO_2)

Ross-Aller solar mix

Sodium
Sodium chloride
Stainless steel

+ Tantalum
Tungsten carbide

Uranium
Uranium dioxide

Water

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*The EOS library is a unique source of data that is utilized internationally. Although it is not a facility research center as others listed in this section, it is included for information purposes.

+Equations of state for these materials were added in the last 12 months.

SECTION E

Summary of Funding Levels

During the fiscal year ending September 30, 1983, the Materials Sciences total support level amounted to about $108.7 million in operating funds (budget outlays) and $8.5 million in equipment funds. The following analysis of costs is concerned only with operating funds i.e., equipment funds which are expended primarily at Laboratories are not shown in the analysis. In contrast, equipment support for the Contract Research projects is included as part of the operating budget.

1. By Region of the Country:

	Contract Research (% by $)	Total Program (% by $)
(a) Northeast..... (Mass., Penn., N.Y., N.J., Del., D.C., Md., Vt., Conn., Me., N.H., R.I.)	47.8	27.8
(b) South..... (Fla., N.C., Tenn., Va., La., Ga., Ky., W.Va.)	9.5	19.6
(c) Midwest..... (Ohio, Ill., Wisc., Mich., Mo., Minn., Ind., Iowa, Kan.)	19.4	31.0
(d) West..... (Ariz., Okla., Wash., Texas, N.Mex., Calif., Utah, Colo., Idaho)	23.3	21.6
	100.0	100.0

2. By Academic Department or Laboratory Division:

	Contract Research (% by $)	Total Program (% by $)
(a) Metallurgy, Materials Science, Ceramics (Office Budget Activity Numbers 01-).....	63.8	40.4
(b) Physics, Solid State Science, Solid State Physics (Office Budget Activity Numbers 02-)....	30.8	49.2

	Contract Research (% by $)	Total Program (% by $)
(c) Chemistry, Chemical Eng. (Office Budget Activity Numbers 03-).....	5.4	10.4
	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, LBL, Ames).....	33.6
(b) DOE Laboratory Programs.....	65.6
(c) Industry and Other.....	0.8
	100.0

4. By Laboratory and Contract Research:

	Total Program (%)
Ames Laboratory	6.6
Argonne National Laboratory	18.4
Brookhaven National Laboratory	19.1
Idaho National Engineering Laboratory	0.4
Illinois, University of (Materials Research Laboratory)	2.7
Lawrence Berkeley Laboratory	7.3
Lawrence Livermore National Laboratory	1.3
Los Alamos National Laboratory	3.4
Oak Ridge National Laboratory	18.0
Pacific Northwest Laboratory	1.8
Sandia National Laboratories	3.0
Solar Energy Research Institute	0.3
Contract Research	17.7
	100.0

6.6
2.7
7.3
17.7
34.3

19240
2935
22175

5. By Selected Areas of Research:

	% of Projects[a] (Total=398)	% of Program Funding[a] ($108.7 million)
Materials		
Ceramics (Crystalline)	31	13.1
Ferrous Alloys	19	7.0
Intermetallics/Hydrides	13	4.9
Polymers	9	2.3
Semiconductors	14	6.3
Technique		
Electron Microscopy (Technique Development)	10	4.0
Neutron Scattering	10	17.7
Synchrotron	8	10.6
Theory	32	9.8
Phenomena		
Catalysis	6	2.4
Corrosion	11	6.4
Diffusion	13	4.0
Processing Science/Synthesis[b]	34	14.8
Strength	12	8.2
Superconductivity	9	4.3
Environment		
High Temperature (> 1200°K)	8	4.8
Radiation	12	13.7
Sulfur-Containing Gases	3	2.1

[a]The summary funding levels 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.

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

MATERIALS

MATERIALS

MATERIALS

TECHNIQUES

TECHNIQUES

TECHNIQUES

TECHNIQUES

PHENOMENA

PHENOMENA

PHENOMENA

PHENOMENA

ENVIRONMENT

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