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Materials Sciences Programs
Fiscal Year 1982

U.S. Department of Energy
Division of Materials Sciences
Office of Basic Energy Sciences
Office of Energy Research
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 Science 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 all research underway in FY 1982 together with a convenient index to the program.

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

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 five sections. Section A contains all Laboratory projects, Section B has all contract research projects, Section C has information on DOE collaborative research centers, Section D shows distribution of funding, and Section E has various indices.

Each project carries a number (underlined) for reference purposes. The FY 1982 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

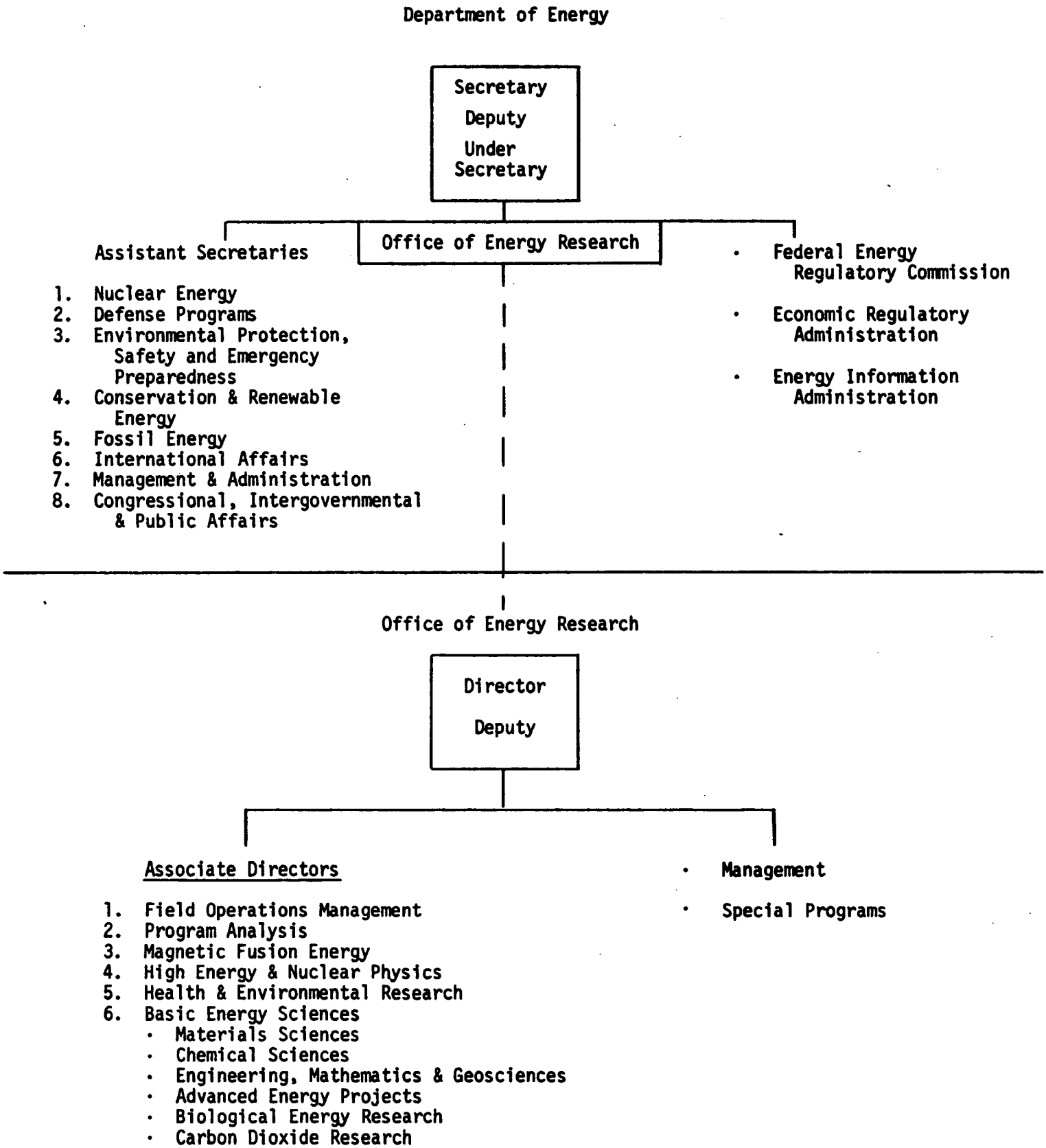
Section C contains information on special DOE centers that are operated for collaborative research with outside participation.

Section D summarizes the total funding level in a number of selected categories. Obviously most projects can be classified under more than one category and, therefore, it should be remembered that the categories are not mutually exclusive.

In Section E the references are to the project numbers appearing in Sections A and B and are grouped by (1) Laboratory investigators, (2) Contract Research investigators, (3) materials, (4) techniques, (5) phenomena, and (6) 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.

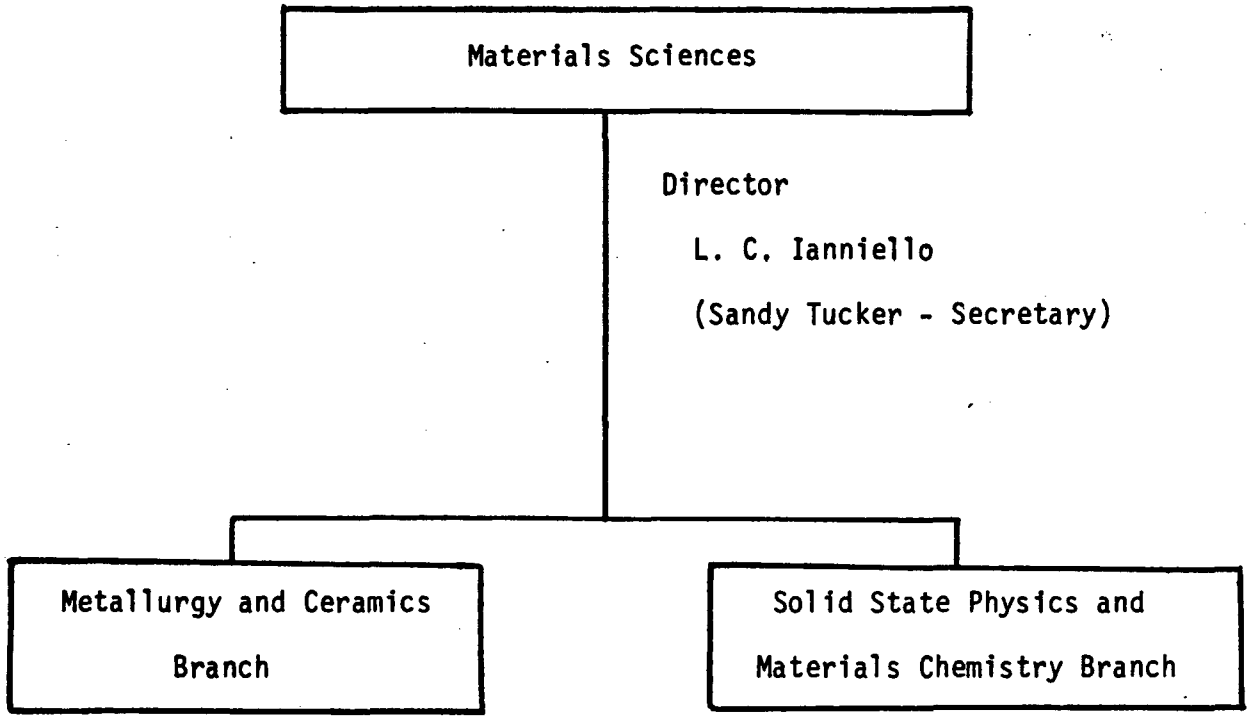
This FY 1982 summary report was coordinated by R. J. Gottschall.


Department of Energy
Secretary
Deputy
Under
Secretary
Assistant Secretaries
1. Nuclear Energy
2. Defense Programs
3. Environmental Protection, Safety and Emergency Preparedness
4. Conservation & Renewable Energy
5. Fossil Energy
6. International Affairs
7. Management & Administration
8. Congressional, Intergovernmental & Public Affairs
Office of Energy Research
• Federal Energy Regulatory Commission
• Economic Regulatory Administration
• Energy Information Administration
Office of Energy Research
Director
Deputy
Associate Directors
1. Field Operations Management
2. Program Analysis
3. Magnetic Fusion Energy
4. High Energy & Nuclear Physics
5. Health & Environmental Research
6. Basic Energy Sciences
• Materials Sciences
• Chemical Sciences
• Engineering, Mathematics & Geosciences
• Advanced Energy Projects
• Biological Energy Research
• Carbon Dioxide Research
• Management
• Special Programs

STRUCTURE OF

DIVISION OF MATERIALS SCIENCES

OFFICE OF BASIC ENERGY SCIENCES



(Janet Venneri - Secretary)

Chief: Vacant
S. M. Wolf
R. J. Gottschall
D. M. Parkin 1/

(Linda Twenty - Secretary)

Chief: M. C. Wittels
T. A. Kitchens
R. H. Bragg 2/
A. C. Switendick 3/
D. T. Cromer 4/
B. C. Frazer 5/
J. B. Darby, Jr. 6/

Notes:
1/ On Leave from Los Alamos National Laboratory
2/ Returning to Lawrence Berkeley Laboratory 8/82
3/ Returning to Sandia National Laboratories - Albuquerque 8/82
4/ Returning to Los Alamos National Laboratory 8/82
5/ On Leave from Brookhaven National Laboratory, arriving 10/82
6/ On Leave from Argonne National Laboratory, arriving 9/82

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SECTION A - Laboratories

SECTION B - Contract Research

SECTION C - Collaborative Research Centers

SECTION D - Funding Levels

SECTION E - Index

SECTION A

Laboratories

This information was provided by the Laboratories. Most projects are of a continuing nature although specific projects were concluded in FY 1982.

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. EMBRITTLEMENT OF 9Cr-1Mo FERRITIC STEELS $ 45,000 01-1
O. N. Carlson

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.

2. MASS TRANSPORT IN SOLIDS $140,000 01-1
O. N. Carlson

Study of diffusion and electrotransport of fast diffusing solutes in yttrium and scandium. Measurement of transport parameters for iron, cobalt and nickel as a function of temperature and determination of activation energy for diffusion. 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.

3. SURFACES AND SOLIDIFICATION $165,000 01-1
R. Trivedi and J. T. Mason

Theoretical 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 cellular to dendritic to eutectic structure. Experimental work on primary dendrite spacing and eutectic spacing in Pb-Sn, Pb-Au and Pb-Pd systems. Study of morphological development in prototype transparent material such as succinonitrile and acetone mixture. Microstructure development during amorphous to crystalline transition.

5236
Rick Schmidt

AMES LABORATORY (continued)

4. CONTROLLED MICROSTRUCTURES — $265,000 — 01-1
J. D. Verhoeven, E. D. Gibson, F. C. Laabs

Production of Nb_3Sn-Cu superconducting composite wire by the in situ process: optimization of J^c and ac loss properties through structure control, factors controlling the reliability of the Sn diffusion process, control of Nb_3Sn grain size, determination of the cause of flux pinning in these materials, development of a cryo-stabilized wire utilizing rolling techniques. A study of directionally transformed pearlite versus temperature gradient, off-eutectoid compositions and applied stress. Preparation of composite Cu-Fe alloys by an in situ casting/mechanical reduction technique and evaluation of structure dependence of resistivity/strength ratio.

5. MECHANICAL METALLURGY AND MATERIALS RELIABILITY — $360,000 — 01-2
O. Buck, C. V. Owen, D. K. Rehbein, B. J. Skillings

Effects of hydrogen on crack initiation in refractory alloys under uniaxial and cyclic loading conditions. Internal friction and acoustic emission studies due to hydrogen in solid solution and due to hydrides. 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 — $ 65,000 — 01-2
M. S. Wechsler

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 — $100,000 — 01-2
M. S. Wechsler

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. Applications to: (1) electron-phonon interactions and charge density waves, (2) shape memory heat engines, and (3) transformation toughening.

AMES LABORATORY (continued)

8. DIFFUSION IN CERAMICS — $145,000 — 01-3
M. F. Berard and G. W. Jordan

Studies of cation self-diffusion and interdiffusion, electrical conductivity (employing impedence spectroscopy), defect structure, and phase equilibrium relationships in fluorite structure binary and ternary single crystal and polycrystalline alloys based on HfO_2 or ZrO_2 which contain Y_2O_3 or rare-earth oxides.

9. RARE EARTH MATERIALS — $400,000 — 01-3
K. A. Gschneidner, Jr., B. J. Beaudry, O. D. McMasters

Preparation and measurement of the superconducting transition temperatures of $La_3(Se_{1-x}S_x)_4$ and $(La_{1-x}Th_x)_3S_4$ alloys. The low temperature (1 - 20 K) - high magnetic field (0 - 10 T) heat capacity study of lattice instability, electron concentration and size effects in rare earth based superconductors: La_3S_{4+x}, La_3Se_{4+x} and $(La_{1-x}Th_x)_3S_y$ ($4 \leq y \leq 4.5$). Study of magnetic phenomena and the quenching of spin fluctuations in (1) highly enhanced paramagnets $LuCo_2$ and $ScCo_2$, (2) metamagnets $CeSn_3$, YCo_2, Sc, and Pd-Ni alloys, and (3) itinerant ferromagnetics Sc_3In and $ZrZn_2$ by low temperature (1 -20 K) heat capacity measurements in magnetic fields up to 10 T.

10. TRANSFORMATION STUDIES AND ORDERED ALLOYS — $110,000 — 01-3
F. X. Kayser

Present studies include (1) determination of the defect contribution to the mass density of high-purity iron-carbon alloy specimens quenched to martensite and retained austenite, and (2) the computer modeling of atomic distributions (cluster models) believed to be present, for example, in dilute Fe-Al, Fe-Si, Cu-Au, and Ni-Mo alloys and the effects of these clusters on electrical, mechanical, and elastic properties.

11. HYDROGEN IN METALS — $235,000 — 01-3
D. T. Peterson

Diffusion, thermotransport, partial molar volume and solubility of H and D in V alloys with Ti, Cr, Nb or O. Photoelectron spectroscopy, optical properties and metallography of metal hydrides and solid solutions.

12. THERMODYNAMICS AND PHASE EQUILIBRIA — $ 45,000 — 01-3
J. F. Smith

Thermodynamic functions for the formation of alloys are being determined by both hydrogen vapor pressure and EMF techniques. Interest currently is in refractory metal systems, e.g., Nb-Ta, and in Y-Fe, Y-Co, and Y-Ni; the latter are glass formers and are also of interest in testing a new theoretical model.

AMES LABORATORY (continued)

13. ULTRASONIC MEASUREMENTS $ 40,000 01-3
J. F. Smith and R. B. Thompson

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. Additional measurements of ultrasonic wave velocities are being measured in Nb with (a) unstressed material, (b) stressed material, (c) plastically deformed material, and (d) annealed material in an effort to quantitatively determine residual stress levels.

14. CERAMIC PROCESSING $135,000 01-5
M. Akinc, M. D. Rasmussen

Influence of preparative procedures on characteristics of precursors and resulting oxides. Surface electrochemical properties of precipitated particles in the aqueous media. Effect of drying methods (oven drying, spray drying, freeze drying, acetone-toluene-acetone drying) on the state of agglomeration. Surface physical and chemical characterization of the precursors, powder morphology sinterability.

15. METALLURGY AND PROCESSING OF REFRACTORY AND STRATEGIC MATERIALS $190,000 01-5
F. A. Schmidt

Improved processing of refractory and strategic metals of interest in present and advanced energy systems. New process being developed for preparing kilogram quantities of high purity vanadium. New techniques will be developed for processing thorium from ThF_4 and for the refining of cobalt metal. Development of arc melting procedure for preparing Cu-Nb alloys containing uniform dispersion of niobium filaments for use in the preparation of superconducting Cu-Nb_3Sn composite wire by the in situ process. 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. New studies concerning solidification of Pd-Cd alloys at extremely high velocity in which the temperature gradient across the solid-liquid interface will be determined.

AMES LABORATORY (continued)

16. NDE MEASUREMENT TECHNIQUES $210,000 01-5
R. B. Thompson, L. W. Schmerr,
L. W. Zachary

Techniques to measure failure related material properties are investigated. Dual objectives of using techniques to improve reliability of inspection and to deepen understanding of failure mechanisms. Ultrasonic scattering techniques to study effects of crack closure on crack growth rates and detectability in aluminum and steels. Acoustoelastic techniques to measure residual stresses in materials with preferred grain orientations. Experiments to investigate relationship of ultrasonic harmonic generation to microcrack distributions and other property degradations occurring during early stages of fatigue.

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

17. NEUTRON SCATTERING $340,000 02-1
W. A. Kamitakahara, C. Loong
C. Stassis, J. Zarestky

Study of the lattice dynamics, thermodynamic properties and structural transformations of metals at high temperatures (Zr, Re, La, Tc); 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 ($CeSn_3$, $CeIn_3$, $CePd_3$); relation of electron-phonon interaction to superconductivity (La,$LaSn_3$).

18. SEMICONDUCTOR PHYSICS $200,000 02-2
A. J. Bevolo, H. R. Shanks,

Preparation and characterization of r.f. sputtered hydrogenated amorphous silicon, amorphous silicon carbide; study of Schottky barriers; measurement of gap states. Electrical resistivity, Hall effect, photoemission, Auger, ELS, and SIMS studies of surfaces and interfaces: metal-semiconductor interfaces (Si on transition metals, rare earths on silicon), Fe-B based amorphous alloys, tin and its oxides, sulfidation of iron-based alloys, corrosion inhibitors on copper, oxygen role in redox reactions on platinum electrodes, and diffusion in ceramics.

AMES LABORATORY (continued)

19. SUPERCONDUCTIVITY $370,000 02-2
D. K. Finnemore, J. E. Ostenson, E. L. Wolf, T. P. Chen, S. Nagata, H. J. Tao

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 14 Tesla range; practical studies to improve wire fabrication techniques and performance characteristics such as critical currents and ac losses.

20. OPTICAL AND SPECTROSCOPIC PROPERTIES OF SOLIDS AND LIQUIDS $320,000 02-2
D. W. Lynch, C. G. Olson, D. M. Wieliczka, J. Kester

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. Photoemission into liquid electrolytes, electrochemical modulation spectroscopy, surface Raman scattering, and photoelectrochemistry on binary alloys susceptible to localized corrosion (benzotriazole on Cu). Surface excitation, and adsorption phenomena on model systems (e.g., noble metals). Photoelectrolysis employing layered compounds. Crystal field and Zeeman spectra of rare earth ions in crystals.

AMES LABORATORY (continued)

21. NEW MATERIALS AND PHASES $420,000 02-2
R. N. Shelton, C. A. Swenson, R. G. Barnes, M. S. Anderson, P. Klavins, D. R. Torgeson, M. L. S. Garcia

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

22. MATERIALS FOR HYDROGEN STORAGE $170,000 02-2
R. G. Barnes, J. D. Corbett, K. A. Gschneidner, Jr., W. A. Kamitakahara, D. T. Peterson, H. Marek, C. K. Saw, R. J. Schoenberger

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.

AMES LABORATORY (continued)

23. X-RAY DIFFRACTION PHYSICS $190,000 02-2
J.-L. Staudenmann

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 $310,000 02-3
B. N. Harmon, K.-M. Ho
M. Luban, D. Misemer, M. Nolan

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. 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). Renormalization group studies of phase transitions.

25. OPTICAL AND SURFACE PHYSICS THEORY $140,000 02-3
R. Fuchs, K.-M. Ho

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. Solar energy studies: electrochemical photovoltaic cells, photolysis, high-temperature adsorbers, and optical properties of phase-change materials for solar applications.

AMES LABORATORY (continued)

26. SUPERCONDUCTIVITY THEORY $120,000 02-3
J. R. Clem, V. Kogan

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; behavior of arrays of nonparallel vortices; critical currents and flux pinning in inhomogeneous superconductors; instabilities; ac losses; superconductivity and magnetic ordering in ternary rare earth compounds (Chevrel phases); the influence of reduced dimensionality on the superconducting properties of highly anisotropic systems; new mechanisms for superconductivity in linear conductors; triplet superconductivity and its physical properties.

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

27. X-RAY AND NEUTRON CRYSTALLOGRAPHY $180,000 03-1
R. A. Jacobson, B. J. Helland

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.

28. METAL-METAL BONDING IN SOLID STATE MATERIALS $170,000 03-1
J. D. Corbett

Materials preparation and characterization of new types of reduced inorganic compounds stable at high temperature (e.g., of Sc, 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 (e.g., of Tl, Ge, Sn, Sb, Bi); ionic intermetallic phases; crystal structures; photoelectron spectroscopy; electronic structure; chemistry of oxygen removal from metals via oxyhalide formation.

AMES LABORATORY (continued)

29. CHEMISTRY OF HEAVY TRANSITION METALS $160,000 03-1
R. E. McCarley

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.

30. METALS FROM FLY ASH $165,000 03-2
G. Burnet, M. J. Murtha

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; utilization of ash processing wastes for cement manufacture.

31. PARTICULATE PROCESSING $275,000 03-2
L. E. Burkhart, A. Cahill

Transport near interfaces, especially drops, bubbles, and solid particles; kinetics and control of particle size distribution, growth rate, and morphology in both liquid phase and vapor phase operations involving the preparation of ceramic powders (yttria, urania, titania); reaction kinetics and mixing in multicomponent mass transfer systems involving chemical reactions with emphasis on correlation between theory and experiment (metal recovery processes)

32. HIGH TEMPERATURE CHEMISTRY $228,000 03-3
H. F. Franzen, Bernd Harbrecht

Structure and bonding in refractory and corrosion-resistant compounds, particularly metal-rich transition metal chalcogenides (ScS), phosphides and aluminides (Zr-Al, Nb-Al, Mo-Al); stability, phase equilibria, X-ray diffraction, photoelectron spectroscopy, and mass spectrometry studies at high temperatures; band structure and electronic properties of transition-metal sulfides.

AMES LABORATORY (continued)

33. SURFACE CHEMISTRY AND CATALYSIS $302,000 03-3
R. S. Hansen, K. G. Baikerikar,
D. C. Johnson

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).

Wiedenbeck - 972-5070
Fradin - -4925
Cafasso - -4542
Lander - -5518
Lam - 4966

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

Materials Science 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

34. ALLOY PROPERTIES $1,140,000 01-1
D. J. Lam, A. T. Aldred,
A. J. Arko, S. K. Chan,
G. S. Knapp, M. V. Nevitt,
B. W. Veal, K. I. Kumagai,
Q. Q. Zheng.

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 (both XANES and EXAFS) spectroscopic studies of structural and electronic properties of various metal oxides in silicate glasses; 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 and inelastic neutron scattering measurements; theoretical studies of electron spectra and bonding of ABO_4 and AB_2O_4 compounds; 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 (both UPS and XPS) studies of actinide intermetallic compounds to determine the electronic configuration and stability of 5f electron states; magnetization, nuclear magnetic resonance and heat capacity studies of local moment interaction in ternary superconductors. Experimental and theoretical studies of the relationship between microscopic lattice properties and electronic properties to the superconductivity of AB_2 intermetallic compounds.

35. SCATTERING STUDIES $ 403,000 01-1
J. Faber, Jr., J. E. Epperson,
T. M. Sabine, H. Shaked,
M. H. Mueller

Structural and dynamic properties of nonstoichiometric oxides, metallic alloys and metal hydrides; emphasis on defect configurations in transition metal oxides; alloy decomposition, local atomic ordering and precipitation in Ni-Al; bonding in ABO_4 compounds; lattice anharmonic effects in AB_3 compounds; experimental studies using neutron and x-ray scattering techniques, both high-angle diffuse, Bragg measurements and small angle. Major involvement with instrument design at the Argonne Intense Pulsed Neutron Source; group is responsible for small-angle neutron scattering prototype and for the general purpose powder diffractometer at IPNS and has major interest in the single crystal instrument for elastic scattering studies, and time-of-flight chopper

ARGONNE NATIONAL LABORATORY (continued)

spectrometers for inelastic studies; development of x-ray diffuse scattering instrumentation for midwest-materials science participating research team at the National Synchrotron Light Source.

36. SURFACE AND THIN FILM STUDIES — $ 453,000 — 01-1
M. B. Brodsky, S. D. Bader, H. C. Hamaker, G. H. Zajak, Y. Zak.

Correlation of electronic structure information on high-density-of-states metal and intermetallic compound surfaces as determined by photoemission spectroscopy, Auger line-shape analysis; and theoretical calculations. Modification of electronic structure by chemisorbed gases, e.g., CO and O_2 and physisorbed gases, e.g., Xe. Surface segregation of alloys, e.g., Ni-Cr; surface magnetism. Modification of materials properties in epitaxial metal film sandwiches, including magnetic and superconducting properties at interfaces; LEED, ELS; XPS; UPS; surface vibrations; low-temperature experiments.

37. STRENGTH AND DEFORMATION OF MATERIALS — $ 391,000 — 01-2
A. P. L. Turner, G. Gottstein, U. F. Kocks, S. R. MacEwen, J. L. Routbort.

Investigation of the mechanisms of deformation and mechanical strengthening in metals and ceramics; neutron diffraction measurements using IPNS of residual stresses produced by deformation of anisotropic polycrystalline materials and their relationship to the Bauschinger Effect; theoretical and experimental investigations of solute hardening and dynamic strain aging; deformation behavior at large strains, including plastic instability and forming limits.

38. METAL PHYSICS — $1,172,000 — 01-3
R. W. Siegel, R. Benedek, M. J. Fluss, N. Q. Lam, J. N. Mundy, L. C. Smedskjaer, D. G. Westlake, B. Chakraborty, T. L. Marcuso, S. Mantl, P. Regnier

The nature and physical properties of atomic defects and their interactions in solids; the atomic mechanisms of diffusion in solids; the nature and properties of metal-hydrogen systems, including the hydrides of intermetallic compounds; investigations of atomic and defect diffusivities, equilibrium defect concentrations, atomic defect interactions with one-another, with solute atoms, and with dislocations, surfaces and interfaces; studies of metals, including bcc refractory metals, alloys, intermetallic compounds, hydrides and glasses, using positron annihilation spectroscopy, radiotracer diffusion, resistometry, electron and field-ion microscopy, electron-energy-loss spectroscopy, neutron and x-ray diffraction, ion-scattering spectroscopy, backscattering spectroscopy and nuclear reaction depth profiling, with a complementary theoretical program utilizing molecular statics and dynamics, computer modelling, and band-structure techniques.

ARGONNE NATIONAL LABORATORY (continued)

39. BASIC CERAMICS $ 471,000 01-3
N. L. Peterson, W. K. Chen,
H. Jain, K. L. Merkle,
J. Sasaki, D. Wolf

Diffusion mechanisms and point defect studies in metal oxides as a function of oxygen pressure at high temperatures using tracer diffusion, conductivity, ion beam scattering and TEM techniques; defect-solute interactions and defect clustering in oxides; theoretical studies of kinetic processes in off-stoichiometric metal oxides; TEM studies of dislocation structures of grain boundaries in oxides; theory of defect kinetics and atomic structures in grain boundaries; grain-boundary diffusion in metal oxides; diffusion mechanisms and impurity interactions in mixed alkali-silicate and borate glasses; oxidation processes in non-stoichiometric oxides using the environmental cell in the HVEM; preparation of single and bicrystals of metal oxides.

40. NEUTRON IRRADIATION STUDIES $ 490,000 01-4
T. H. Blewitt, R. C. Birtcher,
M. A. Kirk, Jr., B. A. Loomis.

Fast neutron irradiation effects in solids studied using the Radiation Effects Facility at IPNS; the structure and properties of interstitials, vacancies, and cascades in metals and ordered alloys investigated with stored energy, resistivity and TEM; radiation embrittlement in ferritic steels and hardening in fcc metals; dislocation interactions studied in the HVEM in niobium, stainless steels and ferritic steels; low temperature defect production and annealing in semiconductors studied with resistivity and deep level transient spectroscopy; superconductors, stabilizers and insulators are studied during low temperature fast neutron irradiation.

41. KINETICS STUDIES $ 851,000 01-4
H. Wiedersich, R. S. Averback,
P. R. Okamoto, L. E. Rehn,
Z. Wang, N. J. Zaluzec.

Investigations into mechanims that lead to the formation of defect aggregates, precipitates and other inhomogeneous distributions of atoms in solids without and with displacement-producing irradiation; surface layer modification of alloys by ion implantation and sputtering; displacement mixing; solute segregation to internal and external defect sinks; effects of irradiation on ordered alloys and on the microstructure of two-phase alloys; in-situ studies of ion and electron irradiation and ion implantation in the High Voltage Electron Microscope; analytical microscopy; radiation sources include HVEM-2MV Tandem facility, 4 MV Dynamitron, and 300 keV ion accelerator.

42. HIGH VOLTAGE ELECTRON MICROSCOPE TANDEM FACILITY $ 535,000 01-4
A. Taylor

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

ARGONNE NATIONAL LABORATORY (continued)

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.

43. MECHANISMS OF FAILURE IN MATERIALS $ 172,000 01-5
A. P. L. Turner, J. L. Routbort

Investigations of the mechanisms of particle impingement erosion of ceramics and corrosion product scales emphasizing the relationships between microstructure, and mechanical properties to erosion behavior. Investigation of the effect of stress on the development of radiation microstructure in the HVEM and its relationship to radiation induced creep.

44. CORROSION STUDIES $ 572,000 01-5
N. L. Peterson, D. J. Baxter,
K. Hoshino, W. E. King,
P. Marikar, K. Natesan,
S. J. Rothman, J. Sasaki

Point defects and diffusion mechanisms in protective oxide scales; grain-boundary diffusion in pure and doped protective oxide materials; sulphur diffusion in oxides; studies of adhesion and morphology of oxide scales and mechanisms by which rare earth alloy additions influence scale adhesion using analytical electron microscopy techniques; mechanisms and kinetics of oxide film breakdown in bioxidant atmospheres.

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

Solid State Science Division - 02 -
P. D. Vashishta - Phone (FTS) 972-5493 or 312-972-5493

45. NEUTRON SCATTERING RESEARCH $710,000 02-1
T. Brun, G. Felcher, J. Jorgensen,
D. L. Price, S. Sinha, R. Kleb, M. Misawa

Use of neutron scattering and diffraction techniques in the study of the properties of condensed matter; instrumentation development and construction in support of the Intense Pulsed Neutron Source and of user activity at that facility; instrumentation responsibility for high-resolution powder diffractometer, crystal analyzer spectrometer, chopper spectrometer, and developmental work on polarized neutron spectrometers. Current areas of research interest include structural and dynamical studies of solid electrolytes, diffraction studies of ternary superconductors, studies of phase transitions in physisorbed monolayer films, investigations of surface magnetism and studies of covalent glasses.

46. MATERIALS PREPARATION AND CHARACTERIZATION $268,000 02-2
S. Susman, D. Hinks

Preparation of metal, insulator and semiconductor single crystals with documented physical and chemical properties; investigations of mechanisms involved in purification and single crystal growth. Materials of current interest are related to studies of fast ion transport in solids, ternary superconductors, systems which display itinerant magnetism, and non-crystalline, inorganic solids.

47. RADIATION EFFECTS IN INSULATORS $133,000 02-2
W. Primak

Studies of defects in insulators involving the damage caused by X-rays, γ-rays, neutrons and charged particles, and the relation of such defects to the transport of ions, atoms and electrons. Major areas of activity include radiation induced dimensional changes and stress relaxation of glasses in high radiation level environments; investigations of glasses in connection with their use as waste storage media and diagnostic windows in fusion reactions, and relationships of radiation damage to radiation dosages.

ARGONNE NATIONAL LABORATORY (continued)

48. SUPERCONDUCTING AND NOVEL MATERIALS $535,000 02-2
C. M. Falco, K. E. Gray, R. Kampwirth,
I. Schuller, C. Chun, M. Kahn,
J. Zasadzinski

Research in fundamental non-equilibrium processes in superconductors and in novel materials, especially with superconductors prepared by sputtering techniques. Current topics include: the preparation and characterization of high T_c materials by high-rate sputtering, layered ultra-thin coherent structures, transport property measurements, thin film magnetic superconductors. A number of applied projects, including the current effort on geophysical prospecting using SQUIDs, have grown from this program.

49. CATALYTIC MATERIALS $445,000 02-2
B. M. Abraham, L. Iton, K. Miyano
T. I. Morrison, T. Tokuhiro

Research investigating the physical and chemical processes occurring at surfaces and interfaces. Research areas include properties of adsorbates on catalytic surfaces such as zeolites, supported metal catalysts and Ziegler-Natta polymerization catalysts; investigations of the rigidity, permeability and ordering of monolayers spread on water; and two-dimensional phase transitions using freely suspended films and monolayers. Experimental techniques include shear measurements of monolayers, resonance methods such as NMR and EPR, and structural techniques such as EXAFS.

50. ELECTRONIC AND MAGNETIC PROPERTIES $695,000 02-2
G. W. Crabtree, B. Dunlap, W. Joss,
H. Kierstead, P. Roach, G. Shenoy,
Y. Takano, A. Umarji

Studies ofelectronic and magnetic properties of solid materials using Mössbauer spectroscopy, de Haas-van Alphen measurements, EXAFS techniques, magnetization and susceptibility measurements and thermodynamic studies. Current research interests include: studies of ternary superconductors having both magnetic and superconducting properties; studies of narrow band materials with an emphasis on mixed valence systems, and a strong interaction with theoretical band-structure calculations; studies of hydrides of intermetallic compounds; studies of the properties of materials at very low materials, currently emphasizing the nuclear magnetic ordering in solid ^{3}He; EXAFS studies of matrix isolated molecules and metal clusters.

ARGONNE NATIONAL LABORATORY (continued)

51. BASIC STUDIES OF SOLAR MATERIALS $144,000 02-2
J. McMillan

Properties of amorphous silicon, chemically modified with hydrogen or fluorine, concentrating on the correlation of structure, stability, degree of modifier incorporation and optical properties with one another and with preparation procedures.

52. FAST ION TRANSPORT IN SOLIDS $250,000 02-2
T. Brun, C. Delbecq, S. Susman

Studies of basic mechanisms for ionic transport of solid electrode and electrolyte materials, utilizing neutron diffraction, nuclear magnetic resonance, molecular dynamics calculations and phonon structure calculations. Current areas of emphasis include: studies of mixed electronic and ionic conductors, currently concentrated on Li-Al alloys; crystalline three-dimensional ionic conductors having framework structures similar to those of the NASICON family; vitreous ionic conductors exhibiting high ionic conductivities.

53. SOLID STATE THEORY AND COMPUTER SIMULATION $560,000 02-3
L. Guttman, R. Kalia, D. Koelling,
A. Rahman, D. Smith, P. Vashishta, A. Fedro

Molecular dynamics and computer simulation of solids and liquids; electronic structure and properties of metals and intermetallic compounds; computer modelling of amorphous systems; many-body effects in semiconductor systems. Current topics include: molecular dynamics calculations to model phenomena such as structural phase transitions, melting and nucleation and fast ion transport in solids; electronic structure calculations of narrow-band materials such as actinides and mixed valence systems; studies of the properties of electron-hole liquids in Ge and Si under various stress situations; development of methods of optical data analysis based on modern dispersion theory; calculations of the crystalline and electronic structure of amorphous semiconductors.

54. DEVELOPMENT OF SYNTHESIS GAS CATALYSTS $60,000 02-5
L. Iton

Development of new catalysts, which are composites of Group VIII metals and molecular shape-selective zeolites, to effect conversions of synthesis gas to low molecular weight olefins.

ARGONNE NATIONAL LABORATORY (continued)

55. GEOPHYSICAL PROSPECTING WITH SQUIDs $200,000 02-5
C. M. Falco, C. W. Lee, R. T. Kampwirth, I. K. Schuller

Development of instrumentation and data analysis techniques for location of subsurface hydrocarbon deposits using Superconducting Quantum Interference Devices (SQUIDs).

Intense Pulsed Neutron Source Program - 02

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

56. PULSED NEUTRON SOURCE OPERATION $ 4,400,000* 02-1

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

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 instruments 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. Approximately 50 experiments, many involving participants in collaborative research from Universities and industry were performed in the period October 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, Solid State Science and Chemistry Divisions of Argonne National Laboratory.

* Support distributed as follows:

01-04	1,500,000
02-01	2,170,000
03-01	730,000
	4,400,000

ARGONNE NATIONAL LABORATORY

Chemical Engineering Division - 03 -
F. Cafasso - Phone: (FTS) 972-4542 or 312-972-4542

57. THERMODYNAMICS & CORROSION CHEMISTRY $835,000 03-02
M. Blander, P. A. G. O'Hare, M.-L. Saboungi, G. Johnson, L. Curtiss, D. Frurip, E. Veleckis, W. Calaway, W. Hubbard, F. A. Cafasso, R. Yonco

Theoretical and experimental investigations of the thermodynamic, thermophysical, constituitive, and corrosion properties of inorganic materials; derivation and testing of theories of high-temperature multicomponent solutions and vapor molecules. Quantum mechanical and statistical mechanical calculations. Calorimetric, electromotive force, vapor pressure, electrical conductivity, solubility, and spectroscopic measurements of condensed gaseous substances having applications in energy-related technologies. Ab initio and semi-empirical studies of the energetics and structure of molecular complexes; thermodynamics of ionic alloys and binary alloy hydrides; thermochemistry of inorganic sulfides and actinide compounds; synthesis and characterization of metastable (amorphous) materials by vapor phase condensation. Liquid metal catalysis. Spectroscopic investigations of aqueous corrosion processes.

58. CHEMISTRY OF MATERIALS $500,000 03-02
R. Kumar, B. Holt, D. Drapcho, S. Johnson

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; phase equilibria in SO_x-NO_x-H_2O-NH_3 systems; heterogeneous and homogeneous conversion chemistries of atmospheric, nitrogen-bearing pollutants; gas solid reaction kinetics.

59. ELECTROCHEMISTRY OF ENERGY SYSTEMS $655,000 03-02
M. Blander, V. Maroni, C. Melendres, Z. Nagy, M.-L. Saboungi, L. Curtiss, J. Settle, R. Yonco

Research on kinetics and mechanisms of processes occurring at cell electrodes and in electrolytes. Surface and interfacial reaction chemistry in electrochemical systems; electrocatalytic reduction of oxygen by transition metal organometallic compounds; electrochemical corrosion and passivation mechanisms; electrodeposition and electrodissolution of metals; electrochemical, spectroscopic (Raman, electronic absorption) surface chemical and theoretical (quantum mechanical) investigations. Ligand field theory and structural chemistry of low-melting organic electrolytes (LMOE); molecular dynamic studies of the structure and energetics of ordered ionic liquids and of colomb complexing; extraction and separations chemistry in LMOE and other molten salt electrolytes.

ARGONNE NATIONAL LABORATORY

Chemistry Division - 03 -
F. Cafasso - Phone: (FTS) 972-3691 or 312-972-3691

60. CHEMICAL STRUCTURE: NEUTRON AND X-RAY STRUCTURAL STUDIES — $420,000 — 03-01
J. M. Williams, A. J. Schultz, R. G. Teller, M. Beno

Research on synthesis and structural characterization of new materials, especially synthetic metals having novel electrical properties and catalyst substances exhibiting high catalytic activity. Development of national university-industrial users group at the Intense Pulse Neutron Source. Structure-property relationships for synthetic metals derived from tetramethyltetraselenafulvalene and for hydrocarbon organometallic complexes or molecular hydrides which are catalysts themselves or mimic real catalysts. Operation and improvement of neutron time-of-flight, single-crystal diffractometer for studies at the Intense Pulsed Neutron Source; Crystal structure and diffuse scattering studies with the SCD. Development of new very low-temperature (10 K) X-ray diffraction facility for coupling X-ray and neutron studies.

61. PHYSICAL AND SURFACE CHEMISTRY OF ENERGY SYSTEMS — $620,000 — 03-03
D. M. Gruen, H. E. Flotow, A. R. Krauss, M. Mendelsohn, M. J. Pellin, and G. J. Lamich

Charge-transfer processes at surfaces; effects of surface chemistry on excitation, de-excitation, ionization and neutralization mechanisms of sputtered species. Development of laser fluorescence spectroscopy (LFS) as a new tool for surface chemistry investigations; velocity distributions of sputtered atoms and ions via LFS; influence of monolayer oxygen coverage on the sputtering properties of neutral transition metal atoms in ground and low-lying metastable energy states. Modification of the structure and properties of surfaces and near surface regions by surface energization techniques; mechanisms of surface segregation in alloy systems; mechanisms influencing secondary ion and photon emission. Electronic structure of naked transition metal clusters; laser cryochemistry of metal dimers in noble gas matrices. Structural and thermodynamic properties of metalloid stabilized intermetallic hydrides, particularly of A_3B_3O phases.

ARGONNE NATIONAL LABORATORY.
Chemistry Division - 03 - (Continued)

62. HIGH-TEMPERATURE MATERIALS CHEMISTRY $480,000 03-03
K. D. Carlson, D. T. Hodul,
R. J. Thorn, G. E. Murch, E. G. Rauh

Research on solid state chemistry of high-temperature electronic and ionic conducting materials important in energy conversion and storage system. Relationship between electronic and electrical properties and influence of composition variation on such properties. Computer simulation of fast oxygen ion transport; diffusion in highly defective solids. Investigations of compositionally induced metal-to-insulator transitions in layered transition metal dichalogenides; electronic structure studies by X-ray photoelectron spectroscopy and photoacoustic spectroscopy. Thermodynamic and transport properties of ZrO_2/ThO_2 refractories. Synthesis of metastable and microheterostructured materials by non-equilibrium condensation.

BROOKHAVEN NATIONAL LABORATORY
Upton, Long Island, New York 11972

Corrosion Science Group -01-
J. R. Weeks - Phone: (FTS) 282-2617 or 516-282-2617
M. Suenaga - Phone: (FTS) ~~282-3718~~ 3518 or 516-282-3518

63. INTERGRANULAR STRESS CORROSION $350,000 01-2
H. S. Isaacs, K. Sieradzki, L. C. Newman

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-
M. Suenaga - Phone: (FTS) 282-3518 or 516-282-3518

64. BASIC PROPERTIES OF AMORPHOUS SEMICONDUCTOR MATERIALS $240,000 01-1
P. E. Vanier, R. R. Corderman, F. J. Kampas

Investigations of the growth, structure, and properties of plasma-deposited thin-film amorphous semiconductors. Studies by optical and mass spectroscopy of processes in the plasma and their relation to film growth and defect formation. Studies of film structure and morphology by electron and optical microscopy, positron annihilation, and 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.

65. RELATIONSHIP BETWEEN PROPERTIES AND STRUCTURES $310,000 01-3
D. O. Welch, M. Suenaga, S. Okuda

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

BROOKHAVEN NATIONAL LABORATORY
Materials Science Division -01- (Continued)

66. PHYSICAL METALLURGY OF METAL-INTERSTITIAL SYSTEMS — $420,000 — 01-3
M. A. Pick, J. R. Bethin, S. M. Heald, D. O. Welch

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.

67. MATERIALS FOR ELECTROCHEMICAL ENERGY CONVERSION AND STORAGE — $100,000 — 01-3
W. E. O'Grady

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.

68. PROPERTIES OF DEFECTS IN MATERIALS — $260,000 — 01-4
C. L. Snead, Jr.

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 by 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.

69. EFFECT OF MICROSTRUCTURE AND ENVIRONMENT UPON FRACTURE TOUGHNESS — $ 70,000 — 01-5
D. Gan

Fundamental study of the relationship between microstructure (as determined by electron microscopy) and fracture toughness of structural materials (Ni, solid solution superalloys and commercial alloys); microstructure changes due to fatigue and creep and various environmental atmospheres.

BROOKHAVEN NATIONAL LABORATORY
Department of Physics -02-
V. J. Emery: (FTS) 666-3765 or 516-282-3765

70. MAGNETIC AND STRUCTURAL PHASE TRANSITIONS — $1,005,000 — 02-01
S. M. Shapiro, G. Aeppli, J. D. Axe, K. Motoya, S. K. Satija

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.

71. ELEMENTARY EXCITATIONS AND NEW TECHNIQUES — $1,238,000 — 02-01
L. Passell, B. H. Grier, C. M. Majkrzak, S. Moehlecke, G. Shirane, E. C. Svensson

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.

72. EXPERIMENTAL RESEARCH - X-RAY SCATTERING — $675,000 — 02-02
B. C. Frazer (on leave), Y. Fujii, J. B. Hastings, M. Kaplan, D. E. Moncton, H. Moudden, W. C. Thomlinson, Y. Yoshizawa

Structural dynamic and electronic properties of condensed matter systems studies by x-ray and neutron scattering. Phase transition, particularly in two-dimensional systems. Liquid crystals. Adsorbed gases. Charge-density wave systems. Intercalated graphite systems. Equipment and technique development for NSLS experiments.

BROOKHAVEN NATIONAL LABORATORY
Department of Physics -02- (continued)

73. EXPERIMENTAL RESEARCH - LOW ENERGY PARTICLE INVESTIGATIONS OF SOLIDS — $580,000 — 02-02

K. G. Lynn, A. N. Goland, P. W. Levy, P. J. Schultz, C. L. Snead, Jr. (DEE); A. Vehanen (U. Helsinki); W. J. Kossler (College of William and Mary); A. P. Mills, Jr. (Bell Labs); I. K. MacKenzie (U. Guelph, Canada); M. S. Spergel (CUNY); D. Fischer, L. Granatelli (SUNY, Stony Brook)

Investigations of perfect and imperfect solids by specialized experimental methods; low-energy positron behavior at and near well-characterized metal surfaces and interfaces, positron bulk diffusion, positron trapping in surface states and positronium formation; development of high brightness positron source at the HFBR; positron annihilation in technologically important metals and alloy systems; development of μSR channel at AGS; calculations of extraterrestrial surface compositions.

74. EXPERIMENTAL RESEARCH - ADVANCED MATERIALS SYNTHESIS AND CHARACTERIZATION — $360,000 — 02-02

D. E. Cox, A. N. Goland, A. R. Moodenbaugh

Synthesis, characterization and electrical properties of inorganic materials with emphasis on electrode materials, solid electrolytes, catalysts or superconductors; fundamental phase equilibria and structural studies by x-ray and neutron diffraction; high-temperature oxide preparation and characterization; application of profile refinement methods to complex oxide structures; studies of structure and disorder in high T_c superconductors; energy-dispersive x-ray diffractometry and development of beam line at NSLS monochromator preparation facility for NSLS.

75. THEORETICAL RESEARCH — $610,000 — 02-03

V. J. Emery, R. Bruinsma, J. Davenport, G. J. Dienes, H. Hamber, R. E. Watson, A. Zangwill

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

BROOKHAVEN NATIONAL LABORATORY
Department of Physics -02- (continued)

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.

76. PARTICLE-SOLID INTERACTIONS - RADIATION EFFECTS RESEARCH — $325,000 — 02-04

P. W. Levy, A. N. Goland,
K. G. Lynn, A. Vehanen (U. Helsinki);
C. L. Snead, Jr. (DEE),
K. J. Swyler (DNE)

Experimental studies of radiation-induced defects in synthetic and natural minerals, in situ measurements of optical absorption and radioluminescence during electron bombardment, thermoluminescence of gamma-irradiated quartz and other minerals; theoretical studies of dislocation generation and thermoluminescence kinetics in irradiated nonmetals; radiation effects in metals, alloys and semiconductors studied by positron annihilation techniques; operation of 3-MeV electron accelerator for radiation effects research.

77. ENGINEERING PHYSICS - SURFACE SPECTROSCOPY — $535,000 — 02-05

R. H. Cantor, W. Eberhardt,
M. Strongin, L. L. Weng, D. Wesner

Photoemission using synchrotron radiation, and other important surface sensitive techniques such as LEED, AES, electron and photon stimulated desorption, to study a variety of problems including a) the electronic and geometric structure of surfaces, b) hydrogen on transition metals, c) the direct comparison between organic molecules in the gas phase and on surfaces, d) cooperative effects and phase transitions in absorbate layers on surfaces; construction of VUV beam line for photoemission experiments at NSLS; development of second VUV line and possible infrared line.

78. ENGINEERING PHYSICS - LOW TEMPERATURE SURFACE PHYSICS — $231,000 — 02-05

W. Eberhardt, Z. Ovadyahu,
M. Strongin

Transport properties, localization and electronic structure in disordered systems; energy transfer mechanisms of molecules to surfaces and the relationship to surface electronic structure; small molecules and rare gas atoms on graphite; metallic clusters

BROOKHAVEN NATIONAL LABORATORY
Department of Physics -02- (continued)

on rare gas solids; phase transitions in adsorbed layers; dissociation barriers on surfaces.

National Synchrotron Light Source -01-
J. P. McTague - Phone: (FTS) 666-4966
-7114

79. EXPERIMENTAL RESEARCH - NATIONAL SYNCHROTRON LIGHT SOURCE, OPERATIONS AND DEVELOPMENT — $4,950,000 — -02-02

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

Operations of the National Synchrotron Light Source and Research and Development in support of the facility. 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 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, development of special high flux or high brightness radiation sources such as wigglers, undulators or FEL's 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 X-ray monochromators, mirror systems, and photon detectors.

Keefer 0351

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

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

80. WELDING RESEARCH $265,000 01-5
J. F. Key, H. B. Smartt, J. W. Chan, C. E. Eiholzer

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.

81. ENVIRONMENTAL EFFECTS ON MECHANICAL PROPERTIES OF METALS $105,000 01-5
G. R. Smolik

Corrosion and failure mechanism in environments generic to coal gasification atmospheres. Environmental variables include various oxidation and sulfidation propensities. Alloy 800 microstructure will be varied to provide different grain sizes and carbide concentrations and distributions.

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

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

82. LOCALIZED CORROSION OF PASSIVE METALS $60,000 01-1
R. C. Alkire

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

83. CENTER FOR MICROANALYSIS OF MATERIALS $175,000 01-1
H. K. Birnbaum and J. A. Eades

Materials characterization as part of collaborative research with DOE Laboratories and Universities Programs personnel, carried out in the University of Illinois Center for Microanalysis of Materials.

84. RAPID SOLIDIFICATION PROCESSING $135,000 01-1
H. L. Fraser

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.

85. SEMICONDUCTOR CRYSTAL GROWTH BY ION BEAM SPUTTERING $135,000 01-1
J. E. Greene

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.

86. DYNAMICAL STRUCTURE OF MATERIALS UNDER EXTREME CONDITIONS OF TEMPERATURE AND PRESSURE $75,000 01-1
J. Jonas

High pressure NMR; dynamical properties of disordered solids including lithium graphites, deuterium molybdenum bronzes, undercooled metals. Techniques for high pressure and high temperature.

87. GRAIN GROWTH IN ALUMINA $60,000 01-1
D. S. Phillips

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

ILLINOIS, UNIVERSITY OF
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88. LASER PROCESSING OF MATERIALS SURFACES — $60,000 — 01-1
M. J. Rigsbee and S. H. Risbud

Development of laser processing methods for modification of structure, composition, chemical properties and erosion/wear resistance of metallic and ceramic material surfaces.

89. CHARACTERIZATION OF COAL — $50,000 — 01-1
C. A. Wert

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.

90. HYDROGEN BEHAVIOR IN BCC METALS — $180,000 — 01-2
H. K. Birnbaum — 31901

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.

91. MECHANICAL PROPERTIES OF MATERIALS — $20,000 — 01-2
J. T. Holder

Ultrasonic and mechanical measurements of inter and intragranular micro-fracture, grain boundary sliding, twinning and plastic flow during triaxial deformation of sandstone, limestone and marble. Plasticity and dislocation motion in ice.

92. COUNCIL ON MATERIALS SCIENCE — $50,000 — 01-2
D. Lazarus

Study and analysis of current and proposed basic research programs on materials, and assessment of their relevance to problems of energy utilization.

93. STRUCTURE, CRACKING AND CORROSION OF CERAMIC GRAIN BOUNDARIES — $75,000 — 01-2
S. D. Brown, W. T. Petuskey and A. Zangvil

Effect of impurities on structure and chemistry of regions contiguous to grain boundaries in SiC and Si_3N_4. Fracture strength toughness, creep and corrosion. Structure of AlN-SiC solid solutions.

94. PHYSICAL PROPERTIES OF CERAMIC MATERIALS — $75,000 — 01-2
W. S. Williams

Strength (flow stress) of carbides, borides, nitrides at high temperatures; electron microscope, characterization of defect structures; conductive and chemical properties of carbides; Auger electron spectroscopy and photoelectron spectroscopy for near surface composition and chemical shifts.

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (continued)

95. OXYGEN IN REFRACTORY BCC METALS — $60,000 — 01-3
C. J. Altstetter

Thermodynamics and diffusion of oxygen in BCC refractory metals and alloys using solid electrolyte cells. Atomic distribution using small angle x-ray scattering. Development of statistical mechanical models.

96. DEVITRIFICATION BEHAVIOR IN METAL-CONTAINING SILICATE GLASSES — $80,000 — 01-3
H. Chen

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.

97. SOLID DIELECTRICS — $95,000 — 01-3
D. A. Payne

STEM, Auger and SIMS analysis of boundary conditions in electrical 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 ceramic microstructures. Fabrication of heterostructure electrodes for the photoassisted electrolysis of water.

98. HYDROGEN TRAPPING IN BCC ALLOYS — $50,000 — 01-3
T. J. Rowland

Electronic structure and atomic distributions in BCC refractory metal alloys containing hydrogen. Computer simulation, extended x-ray absorption fine structure, inelastic neutron scattering, conductance nuclear magnetic resonance measurements and powder preparation techniques.

99. MICROWAVE STUDIES OF DISORDERED MATERIALS — $65,000 — 01-3
H. J. Stapleton

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

100. LOW TEMPERATURE STUDIES OF DEFECT STRUCTURE IN SOLIDS — $90,000 — 02-2
A. C. Anderson

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

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (continued)

101. PHOTOEMISSION STUDIES OF THE ELECTRONIC STRUCTURE OF SURFACES AND INTERFACES — $95,000 — 02-2
T.-C. Chiang

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

102. RESPONSE OF SOLIDS TO ELECTROMAGNETIC RADIATION — $105,000 — 02-2
J. D. Dow

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.

103. USE OF VERY HIGH PRESSURE TO INVESTIGATE THE STRUCTURE OF MATTER — $165,000 — 02-2
H. G. Drickamer

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: (1) luminescence properties (2) optical effects at a semiconductor-electrolyte interface.

104. EXCITON COLLECTION FROM ANTENNA SYSTEMS INTO ACCESSIBLE TRAPS — $75,000 — 02-2
L. R. Faulkner

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.

105. IMPURITIES IN SUPERCONDUCTORS — $65,000 — 02-2
D. M. Ginsberg

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

106. ULTRASONIC INVESTIGATIONS OF THE STRUCTURE OF MATTER — $135,000 — 02-2
A. V. Granato

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

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107. DEFECT AND ELECTRONIC PROPERTIES OF SOLIDS — $90,000 — 02-2
D. Lazarus

Atomic mobility in solid electrolytes and metallic glasses. Electrical resistivity and Hall effect in metallic glasses as a function of pressure and temperature.

108. PROPERTIES OF CRYSTALLINE CONDENSED GASES — $135,000 — 02-2
R. O. Simmons

Momentum density in solid helium by neutron scattering; thermal and isotopic point defects in helium crystals; isotopic phase separation in solid helium; elastic constants and phase transitions in solid methanes; quantum effects in diffusion.

109. NUCLEAR MAGNETIC RESONANCE IN SOLIDS — $165,000 — 02-2
C. P. Slichter

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

110. PHYSICAL PROPERTIES OF ORDERED AND DISORDERED SOLID SOLUTIONS — $100,000 — 02-2
H. Zabel

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.

111. PHASE STABILITY, IRRADIATION EFFECTS AND MECHANICAL PROPERTIES OF STAINLESS STEEL — $30,000 — 02-4
J. E. Cunningham, B. C. Muddle, J. C. Stubbins

Synthesis and characterization of thin film stainless steel; equilibrium FeCrNi phase diagram; evolution of alloys under electron irradiation.

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112. STRUCTURE AND PROPERTIES OF TRANSFORMATION INTERFACES — 146,000 — 01-1
R. Gronsky

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.

113. MICROSTRUCTURE, PROPERTIES, ALLOY DESIGN: INORGANIC MATERIALS — 513,000 — 01-1
G. Thomas

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.

114. SOLID STATE PHASE TRANSFORMATION MECHANISMS — 166,000 — 01-1
K. H. Westmacott

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 amd 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.

115. NATIONAL CENTER FOR ELECTRON MICROSCOPY — 700,000 — 01-1
G. Thomas, R. Gronsky,
and K. H. Westmacott

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.

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116. IN-SITU INVESTIGATIONS OF GAS-SOLID REACTIONS BY ELECTRON MICROSCOPY — 65,000 — 01-1
J. W. Evans and K. H. Westmacott

The investigation of in-situ reactions using an environmental cell in the 650 kV and new 1.5 MeV high voltage electron microscopes. Emphasis is on investigation of the effect of microstructure, e.g., dislocations, grain boundaries, and surfaces on reactions between gases and solids. Nickel oxide reduction has been studied by ex-situ and in-situ experiments, and presently the reduction of iron oxides is being investigated. Subsequently, other reactions of significance to materials performance in energy conversion systems will be studied.

117. LOCAL ATOMIC CONFIGURATIONS IN SOLID SOLUTIONS — 60,000 — 01-1
D. de Fontaine

Present study is aimed at capturing the early stages of phase transformations in materials, primarily metallic alloys. Atomic ordering is studied in systems exhibiting the phenomenon of long-period superstructure formation, the theoretical tool being that of various approximations of the Ising model with long-range interactions, the experimental one being high-resolution electron microscopy. Atomic clustering, or phase separation, is studied in alloys exhibiting partitioning of substitutional and interstitial solute, the theoretical tool here being multicomponent nucleation and growth theory, the experimental one being analytical electron microscopy.

118. COLLABORATIVE STUDIES BY TEM — 0 — 01-1
A. W. Searcy

Collaboration between materials scientists, physicists, and chemists in MMRD with TEM specialists; to start in FY 1983.

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119. THEORETICAL PROBLEMS IN ALLOY DESIGN 453,000 01-2
J. W. Morris Jr.

This project is a multifaceted program of research in physical metallurgy that concentrates on the science of alloy development for advanced energy needs. Specific tasks include: 1) theoretical research, which addresses the theory of phase transformations in solids and the influence of microstructure on mechanical properties; 2) experimental research in fundamental metallurgy, which addresses the control of microstructure through thermomechanical processing, and the influence of microstructure on material properties; 3) the development of new structural alloys for use in advanced energy systems, a task which is now particularly concerned with the provision of better structural materials for low-temperature use; 4) welding research, which addresses the development of appropriate combinations of weld metallurgy and welding procedure to maintain toughness in high-strength welded alloys; and 5) high-field superconducting materials, which is concerned with the development of wire manufacturing procedures that permit the use of advanced A15 compounds.

120. MECHANICAL PROPERTIES OF CERAMICS 206,000 01-2
A. G. Evans

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.

121. ENVIRONMENTALLY AFFECTED CRACK GROWTH IN ENGINEERING MATERIALS 76,000 01-2
R. O. Ritchie

The role of microstructure and environment in influencing the propagation of fatigue cracks in ferrous alloys has been examined with specific reference to behavior at ultralow, near-threshold growth rates ($<10^{-6}$ mm/cycle). Experimental observations have indicated that such near-threshold cracks (i) propagate much faster in dry inert gas (i.e., helium or argon) compared to air, (ii) suffer invironmentally accelerated crack growth in hydrogen gas only where the mean (as opposed to cyclic) stresses are low, (iii) are decelerated in hydrogen gas at high strength levels, and (iv) propagate slower in coarser-grained microstructures. Such surprising behavior has been quantitatively modeled using oxide-induced and roughness-induced crack closure mechanisms where the influence of crack face oxidation products and rough fracture morphologies are considered in terms of prematurely wedging the crack closed at positive loads in the fatigue cycle.

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122. INTERFACES AND CERAMIC MICROSTRUCTURES 10,000 01-03
J. A. Pask

Kinetics and mechanisms of solid-state reactions, nucleation and growth phenomena, and distribution of phases in multiphase ceramic systems whose principal phase constituents are within the Al_2O_3-SiO_2 system. Thermodynamic considerations of sintering with a liquid phase.[3] Mechanisms of corrosion of ceramic materials. Thermodynamics and kinetics of electrochemical reactions at glass-metal interfaces.

123. HIGH-TEMPERATURE REACTIONS 260,000 01-03
A. W. Searcy

Recent studies have focused on the thermodynamics and kinetics of decomposition reactions. Emphasis is placed on coupling kinetic studies with measurements of properties of the solid product of decomposition reactions as functions of the temperature, reactant particle size, particle bed size, and product gas pressure. Also under study are vapor transport through porous solids, surface kinetics, and surface and solid solution thermodynamics.

124. STRUCTURE-PROPERTY RELATIONSHIPS IN SEMICONDUCTOR MATERIALS 265,000 01-3
J. Washburn

An investigation of the mechanisms of crystal defect formation associated with processing of Si, GaAs, and other semiconductor materials--effects of defects on electrical properties--emphasis on: 1) ion-implantation phenomena (point defect clustering, precipitation, crystal to amorphous, and amorphous to crystal transformation); 2) structure of the Si-SiO_2 interface; 3) phase changes in $Cu_{(2-x)}S$ associated with degradation of the CdS-$Cu_{(2-x)}S$ solar cell. Primary techniques are: high-resolution lattice-imaging electron microscopy, channeled Rutherford backscattering, secondary ion mass spectroscopy, and electrical measurements.

125. PROPERTIES AND PROCESSING OF REFRACTORY CERAMICS 195,000 01-3
L. C. De Jonghe

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.

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126. STRUCTURE AND ELECTRICAL PROPERTIES OF COMPOSITE MATERIALS — 108,000 — 01-3
R. H. Bragg

Structure, electrical, and thermophysical properties of carbon materials heat treated in the range 1000°C-3000°C. Characterization using x-ray and electron diffraction, electron microscopy, and small angle x-ray and neutron scattering. Measurements of electrical conductivity, Hall coefficient, and magnetoresistance in the range 2.8°K-300°K in magnetic fields of 5 Telsa. Mechanisms of graphitization and point defect annealing in glassy carbon and pyrolytic graphite. Synthesis and characterization of graphite intercalation compounds. Interfaces in carbon fiber reinforced composites. Coal characterization.

127. ASSIGNMENT WITH DOE WASHINGTON — 103,000 — 01-3
R. H. Bragg

Assignment of principal investigator to DOE/BES to assist in the review and evaluation of programs.

128. HIGH-TEMPERATURE OXIDATION AND CORROSION OF MATERIALS — 357,000 — 01-3
D. P. Whittle*

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.

129. CERAMIC INTERFACES — 50,000 — 01-3
A. M. Glaeser

Investigation of grain boundary migration behavior and its effect 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. Determination of the influence of MgO content, driving force, and temperature on migration behavior of individual grain boundaries in Al_2O_3.

*Deceased, 7/23/82

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130. EROSION-CORROSION WEAR PROGRAM 190,000 01-5
A. V. Levy

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.

131. ABRASIVE, EROSIVE, AND SLIDING WEAR OF MATERIALS 75,000 01-5
I. Finnie

Mechanisms of two- and three-body abrasive wear of metals. High-temperature three-body wear testing. Erosive wear as a function of abrasive and material hardnesses. Simulation of sliding wear in larger scale tests. Correlation of sliding wear to mechanical properties.

132. EROSION OF BRITTLE SOLIDS 70,000 01-5
A. G. Evans

This project is concerned with the development of a fundamental understanding of erosion and strength degradation in brittle solids subject to impact by solid particles. The principal research directions involve studies both of the damage created by the impact of individual partaicles and of the erosion characteristics under multiple impact conditions. The studies are conducted as a function of temperature, velocity, angle of incidence, and projectile hardness in order to identify specific mechanisms of erosion and strength degradation. Predictions of erosion are generated for each important material removal mechanism.

133. CHEMICAL DEGRADATION OF REFRACTORIES 55,000 01-5
D. P. Whittle

Thermodynamic, kinetic, and structural factors controlling chemical degradation mechanisms of refractories. Alumina ceramics containing calcia are of primary interest, and the chemical response of the bonding or intergranular phases to high-temperature sulfur-containing environments using thermogravimetry and microscopal techniques is being studied. Refractory/molten slag interactions are also part of the program.

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134. FAR-INFRARED SPECTROSCOPY 202,000 02-2
P. L. Richards

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 physically bound to metal surfaces, the infrared properties of solids with charge-density wave transitions, the far-infrared spectra of organic superconductors, the infrared photoconductivity of impurities in semiconductors, the infrared radiation from dust clouds in our galaxy, and the infrared radiation left over from the creation of the universe.

135. EXPERIMENTAL SOLID-STATE PHYSICS AND QUANTUM ELECTRONICS 238,000 02-2
Y. R. Shen

Development of laser spectroscopic and modern optical techniques for material studies. Applications of these techniques to study linear and nonlinear optical properties of gases, liquids, semiconductors, and metals. Investigation of new phenomena resulting from interaction of light with matter: multiphoton dissociation of molecules, surface electromagnetic wave interaction, surface-enhanced optical effects, surface nonlinear optics, etc. Use of lasers to study current problems of interest: isotope separation, van der Waals molecules, surface phenomena, molecular adsorption and desorption, and interface properties.

136. EXCITATION IN SOLIDS 150,000 02-2
C. D. Jeffries

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 studied in detail. The computed predictions of a one-dimension one-parameter model (the logistic map) are in surprising agreement with the data. The approach to noisy behavior is being studied experimentally, for a wide class of nonlinear phenomena in solids, to test the validity of universal models of routes to chaos.

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137. TIME-RESOLVED SPECTROSCOPIES IN SOLIDS — 60,000 — 02-2
P. Y. Yu

Application of an optical system capable of measuring absorptivity, 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, temporal 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.

138. SUPERCONDUCTIVITY, SUPERCONDUCTING DEVICES, AND 1/f NOISE — 250,000 — 02-2
J. Clarke

Development of Superconducting Quantum Interference Devices (SQUIDs) for measuring voltages 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. Nonequilibrium superconductivity: enhancement of the superconducting energy gap by microwaves and phonons, measurement of the electron-phonon relaxation times in superconductors, generation of charge imbalance by temperature gradients. Study of 1/f noise in SQUIDs and metal films.

139. THEORETICAL STUDIES OF THE ELECTRONIC PROPERTIES OF SOLID SURFACES — 40,000 — 02-3
L. M. Falicov

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).

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140. THEORETICAL SOLID-STATE PHYSICS 60,000 02-3
M. L. Cohen

A microscopic approach is used to explain the observed properties of solids. One objective is to predict electronic, vibrational, and structural properties of solids and surfaces using only properties of the constituent atoms. Quantum mechanical methods are used, and the electron-ion pseudopotential is exploited for many calculations. Specific calculations include: electronic band structure, optical reflectivity and photoemission, surface and interface characteristics, superconductivity, transport, vibrational and structural properties.

141. LOW-TEMPERATURE PROPERTIES OF MATERIALS 140,000 03-01
N. E. Phillips

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.

142. ELECTROCHEMICAL PROCESSES 130,000 03-1
C. W. Tobias

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. Gas-electrolyte-electrode interfaces: supersaturation, coalescence, and bubble separation phenomena. Nonaqueous ionizing solvents: thermodynamic and kinetic properties of electrode reactions which are not feasible in aqueous media.

143. HIGH-TEMPERATURE THERMODYNAMICS 138,000 03-03
L. Brewer

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.

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144. CHEMISTRY AND MATERIALS PROBLEMS IN ENERGY PRODUCTION TECHNOLOGIES — 234,000 — 03-3
D. R. Olander

Chemical and physical behavior of materials in environments characteristic of energy production devices, with major emphasis on fission and fusion reactors. Experiments are designed to develop insight into the mechanisms of the phenomena involved: The high-temperature behavior of uranium dioxide, including transient vaporization, oxygen self-diffusion, thermal gradient migration of inclusions, and hydrogen solubility; molecular beam studies of gas-solid reactions, including hydrogen atom reaction with ceramic oxides and the silane cracking reaction; stress corrosion cracking of zircaloy; brine inclusion migration in salt.

145. PLASMA-ENHANCED DEPOSITION OF THIN FILMS — 50,000 — 03-3
D. W. Hess

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.

146. ELECTROCHEMICAL PHASE BOUNDARIES — 158,000 — 03-3
R. H. Muller

Formation of boundary layers at electrochemical interfaces and control of mass transfer processes. Solid and liquid thin films at electrodes, nucleation and growth processes, effect on electrochemical reactions, control of film properties. Electrodeposition and dissolution of metals. Development and use of optical techniques for the characterization of surfaces in liquid media.

147. SOLID-STATE AND SURFACE REACTIONS — 332,000 — 03-3
G. A. Somorjai

The research program is centered on studies of catalyzed surface reactions and 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, rhenium, molybdenum, metals and their compounds, and bimetallic alloys. The adsorbates and reactants are mostly hydrocarbons, oxygen, hydrogen, and water.

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148. NUCLEAR MAGNETIC RESONANCE 148,000 03-3
A. Pines

The primary objective is to develop new magnetic resonance spectroscopic techniques 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 vibrations and rotation, and with external excitation by radiofrequency sources and light. Recent novel techniques include multiple quantum spectroscopy, high-resolution nuclear magnetic resonance in solids, and magnetic isotope effects. Applications include the study of molecular conformation and dynamics in several phases, including amorphous solids, ferroelectrics, liquid crystals, polymers, and fuel related materials. Some molecular properties change upon light excitation, and laser magnetic double-resonance techniques are being used to examine how these changes dictate the course of photochemical reactions.

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149. HOT CORROSION STUDIES RELATED TO FOSSIL FUELS — $280,000 — 01-1
J. Truhan, O. Krikorian

Mechanisms and kinetics of hot gas/molten salt-oxide corrosive attack of metals; develop quantitative model to relate the susceptibility of nickel and iron base alloys to corrosive media at elevated temperatures (800° to 1000°C); study of early stages of corrosion; kinetics studied by weight change and scale growth; salt-substrate interactions; molten salt electrochemical reactions.

150. RAPIDLY QUENCHED Al AND Mg ALLOYS — $120,000 — 01-3
L. Tanner, C. Cline

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

151. OPTICAL MATERIALS RESEARCH — $250,000 — 02-2
M. Weber, S. Brawer

Nonlinear optical properties of transparent materials subject to intense light beams and growth and spectroscopy of new laser materials. Intensity-dependent refractive index changes measured using time-resolved laser interferometry. Two-photon absorption at near-ultraviolet to near-infrared wavelengths detected using photoacoustic and photorefractive techniques. Dependence of spectroscopic and optical properties on materials composition. Materials include oxide and fluoride glasses and crystals.

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152. LASER-EXCITED FLUORESCENCE IN AMORPHOUS SOLIDS — $210,000 — 02-2
S. Brawer, M. Weber

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. Simple and multicomponent oxide and fluoride glasses. Experimental spectra are compared with site-dependent fluorescence properties calculated from computer simulations of glass structure using Monte Carlo and molecular dynamic methods.

153. SURFACE PHYSICS AND CHEMISTRY OF LASER INDUCED DAMAGE — $240,000 — 02-2
W. Siekhaus, W. Lowdermilk

Investigation of the fundamental physical and chemical processes 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 absorption 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 μm laser pulses. Multiphoton induced electron emission is monitored along with Auger analysis.

154. D-T CRYOGENIC PROPERTIES — $170,000 — 03-2
P. Souers

Measurement of D_2+T_2 chemical reaction rates in the solid and liquid phases by infrared spectroscopy. Measurement of D_2-T_2 rotational reaction rates by nuclear magnetic resonance. Engineering-type measurements on a DT-He^3 mixture phenomenon that halts the flow of gas into the cryostat. Study of frozen "super-ions" in solid T_2 using infrared spectroscopy. The D_2+T_2 gas phase kinetic experiments using mass spectroscopy. Solid thermal conductivity measurements using nuclear magnetic resonance. Optical absorption spectroscopy of trapped electrons in the solid.

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

Chemistry-Materials Science Division
S. S. Hecker - Phone: (FTS) 843-4563 or (505) 667-4563

155. THE EFFECT OF SELF-IRRADIATION ON STABILITY OF CERAMIC NUCLEAR WASTE — $250,000 — 01-4
F. W. Clinard, Jr., G. F. Hurley, D. E. Peterson, D. L. Rohr

Alpha decay self-damage in zirconolite, perovskite, and SYNROC ceramic waste; doping with short half-life actinides; characterization of damage effects and disorder by x-ray and electron diffraction, electron and optical microscopy, thermal conductivity, dilatometry, and calorimetry; strength and fracture; elevated temperature effects; amorphization by quenching; dependence of damage response on composition and fabrication parameters.

156. MECHANICAL PROPERTIES — $310,000 — 01-5
J. J. Petrovic, M. G. Stout, K. P. Staudhammer

Multiaxial deformation of aluminum, aluminum alloys, titanium, brass, OFHC copper, and 304 stainless steel; yield surfaces and multiaxial stress-strain relations; stress path changes; large strain deformation; multiaxial ductile fracture; geometric instabilities in tubes and sheet; substructural evolution with strain, strain state and strain rate; brittle fracture of Al_2O_3, Si_3N_4, SiC and ZrO_2 under multiaxial stresses; mixed-mode brittle fracture; Weibull statistical fracture theory for multiaxial loading; indentation-produced surface flaws and fracture toughness of ceramics.

157. STRUCTURAL CERAMICS — $146,000 — 01-5
J. J. Petrovic, F. D. Gac, J. V. Milewski, H. Sheinberg, D. E. Hull L. R. Newkirk, C. Hollabaugh

Fabrication-microstructure-properties interrelationships for structural ceramics; fabrication of dense SiC and Si_3N_4 materials without the use of densification additives; SiC and Si_3N_4 ultra-fine/ultra-pure powder production by RF-plasma methods; SiC and Si_3N_4 single crystal whisker growth by vapor-liquid-solid (VLS) techniques; powder activation by shock loading and irradiation; hot-pressing and sintering consolidation; relationships between processing and microstructure, mechanical behavior, and oxidation/corrosion response.

LOS ALAMOS NATIONAL LABORATORY (continued)

158. SURFACE SCIENCE RESEARCH $186,000 03-2
T. N. Taylor, C. T. Campbell
R. W. Springer

I. Surface Modification of Materials: Model Chemisorption Studies. Adatom/substrate combinations from metals and semimetals; selective modification of chemisorption properties by surface additives; electron, photoelectron, and thermal desorption spectroscopies, low-energy electron diffraction and work function measurements; relationship that surface electronic, structural, and compositional factors have to surface reactivity. II. A Study of the Mechanisms of Compound Formation During Deposition. Low-energy ion bombardment of aluminum surfaces; nitride formation during sputtering; current and voltage thresholds for compound formation on clean surfaces; model development for compound formation; low-energy ion range estimates.

1757 Bowman

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

159. THERMOPHYSICAL PROPERTIES OF MATERIALS $180,000 02-2
J. C. Wheatley, M. P. Maley,
A. Migliori, G. W. Swift,
J. J. Haucke, J. Helffrich,
T. J. Hofler, Y. Maeno

Properties of liquids working in heat engines; scientific qualities of Stirling and Stirling-Malone heat engines, heat pumps, and refrigerators using propylene near room temperature; properties of the required "second thermodynamic media", novel approaches to making the liquid medium go through its thermodynamic cycle. Intrinsically irreversible heat engines, especially using acoustical techniques with gases, possible applications to magnetic systems. Helium isotope heat engines which cross the critical region. Heat transfer by diffusive conduction and gravitational convection in dilute solutions of ^{3}He in superfluid ^{4}He. Novel processes of heat transfer in ^{3}He-^{4}He solutions near the tricritical point. Properties of gaseous atomic hydrogen isotopes at low temperatures.

160. ULTRAHIGH-PRESSURE STUDIES OF HYDROGEN $180,000 02-2
R. L. Mills, R. A. LeSar

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

LOS ALAMOS NATIONAL LABORATORY (continued)

161. MATERIALS RESEARCH AT THE WNR/PSR FACILITY — $1,190,000 — 02-1
R. N. Silver, J. Eckert, J. Goldstone, P. Seeger, P. Vergamini, R. Alkire, A. Soper, R. Brugger, A. D. Taylor, and A. Larson

Materials science research by neutron scattering at the WNR/PSR pulsed spallation neutron source. Includes the development of novel time of flight instruments. Inelastic neutron scattering studies of metal hydrides, chemical spectroscopy, elementary excitations in solids, and eV spectroscopy. Neutron diffraction studies of molecular liquids, amorphous materials, powders and single crystals.

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

162. LOS ALAMOS EQUATION OF STATE LIBRARY — $250,000 — 02-3
J. Abdallah, R. C. Albers, B. I. Bennett, F. Dowell, W. F. Huebner, J. D. Johnson, S. P. Lyon

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 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.

163. ELASTIC WAVE SCATTERING AND QUANTITATIVE FLAW AND MICROSTRUCTURE CHARACTERIZATION — $170,000 — 01-5
J. E. Gubernatis, W. M. Visscher

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

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Oak Ridge, Tennessee 37830

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

164. DOE FACILITY USERS PROGRAM $130,000 01-1
A. Wohlpart

This project supports collaborative work between university researchers and national laboratories; one program involves apparatus at ORNL such as the high voltage electron microscope and the analytical electron microscope; the second program involves the National Synchrotron Light Source at BNL.

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

165. THEORETICAL STUDIES OF METALS AND ALLOYS $480,000 01-1
J. S. Faulkner, W. H. Butler, G. S. Painter, G. M. Stocks

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_{C2} 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.

166. STRUCTURE OF COAL $125,000 01-1
L. A. Harris, O. C. Kopp

TEM, SEM, microprobe, optical and infrared petrography of microporosity and micromineralogy of coal macerals; correlation of coal rank with micro-structure; characterization of secondary minerals; anthracite, bituminous, sub-bituminous, and channel coals; in situ studies of maceral-mineral and maceral-maceral reactions using HVEM.

167. X-RAY SCATTERING RESEARCH $530,000 01-1
C. J. Sparks, B. S. Borie, G. E. Ice, H. L. Yakel

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; theoretical studies of extinction phenomena.

OAK RIDGE NATIONAL LABORATORY
Metals and Ceramics Division -01- (continued)

168. HIGH VOLTAGE AND ANALYTICAL ELECTRON MICROSCOPY $420,000 01-1
J. Bentley, E. A. Kenik, P. S. Sklad

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.

169. DEFORMATION AND MECHANICAL BEHAVIOR OF STRUCTURAL MATERIALS $600,000 01-2
M. H. Yoo, J. C. Ogle, J. Schneibel, C. L. White, G. F. Petersen

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.

170. MECHANICAL PROPERTIES OF CERAMICS $470,000 01-2
P. F. Becher, G. W. Clark, M. K. Ferber, C. J. McHargue, C. S. Yust

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.

171. KINETICS AND MECHANISMS OF SURFACE AND SOLID STATE REACTIONS $700,000 01-3
J. V. Cathcart, R. E. Druschel, R. A. McKee, R. E. Pawel

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.

OAK RIDGE NATIONAL LABORATORY
Metals and Ceramics Division -01- (continued)

172. PHYSICAL PROPERTIES RESEARCH $180,000 01-3
D. L. McElroy, R. K. Williams

Development and application of measurement methods for physical property studies from 4.2 to 2600 K; correlation of electronic energy transport through the Lorenz constant; phonon scattering by electrons and defects in refractory metals and alloys (V, Nb, Ta, Cr, Mo, W, Pd) and transition metals (Fe, Ni, Cr); phonon-phonon scattering in insulating solids, effect of cation-anion mass ratio, grain boundaries and crystal structure; properties of LRO alloys.

173. METASTABLE MATERIALS $480,000 01-3
C. C. Koch, A. DasGupta,
D. S. Easton, D. M. Kroeger

Amorphous superconductors based on Mo, Nb, La, and Re with other transition metals and/or metalloids; 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.

174. RADIATION EFFECTS $1,300,000 01-4
L. K. Mansur, W. A. Coghlan, K. Farrell,
M. B. Lewis, N. H. Packan, L. L. Horton,
C. L. White, E. H. Lee

Neutron damage in pure metals and alloys 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, LRO alloys, ferritic alloys. 624- 4804

175. FUNDAMENTAL STUDIES IN WELDING $360,000 01-5
S. A. David, J. M. Vitek

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

OAK RIDGE NATIONAL LABORATORY
Metals and Ceramics Division -01- (continued)

176. RESEARCH IN CERAMIC PROCESSING $275,000 01-5
P. F. Becher, C. B. Finch, C. J. McHargue

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.

OAK RIDGE NATIONAL LABORATORY
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

177. INTERATOMIC INTERACTIONS IN CONDENSED SYSTEMS — $1,420,000 — 02-1
R. M. Nicklow, J. W. Cable, H. R. Child, C. B. Clark, W. C. Koehler, H. A. Mook, R. M. Moon, O. A. Pringle, H. G. Smith, K. Werner

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 $CePd_3$, LaB_6, LaF_3, and intercalated graphite; magnetic excitations in UAl_2, $CePd_3$, and Er; phase transitions in MnP; magnetic form factors of mixed-valence materials; structures of composition modulated systems. ORNL neutron scattering facilities are available to scientists of other organizations through Neutron Users' Program.

178. PROPERTIES OF DEFECTS, SUPERCONDUCTORS AND HYDRIDES — $900,000 — 02-1
R. M. Moon, J. W. Cable, H. R. Child, W. C. Koehler, H. A. Mook, R. M. Nicklow, O. A. Pringle, H. G. Smith, G. D. Wignall

19-8 : 11

Elastic, inelastic, and small-angle scattering of neutrons by superconductors, metal hydrides, and defects in single crystals; lattice dynamics of α-U, A15 compounds, $PdTe_2$; defects in KCl and CaO; proton diffusion in biological systems; magnetic structures in reentrant superconductors; SANS from coal solutions, oil shale, surfactants, and polymer blends. ORNL neutron scattering facilities are available to scientists of other organizations through Neutron Users' Program.

179. SMALL-ANGLE X-RAY SCATTERING — $120,000 — 02-2
W. C. Koehler, J. S. Lin, S. Spooner

Small-angle x-ray scattering of metals, alloys, polymers, and surfactants; void distributions in oil shale and irradiated metals; dynamic deformation studies of polymers.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

180. PHYSICAL PROPERTIES OF CERAMICS — $575,000 — 02-2
F. A. Modine, Y. Chen,
R. R. Gonzalez, G. R. Gruzalski,
T. M. Haywood, J. R. Martinelli,
E. Sonder, R. A. Weeks

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.

181. SOLID ELECTROLYTES AND SUPERIONIC CONDUCTIVITY — $345,000 — 02-2
J. B. Bates, G. M. Brown,
W. E. Brundage, N. J. Dudney,
S. Casey, B. C. Larson,
J. C. Wang

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; 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.

182. PHYSICAL PROPERTIES OF SUPERCONDUCTORS — $430,000 — 02-2
S. T. Sekula, B. R. Appleton,
D. K. Christen, H. R. Kerchner,
J. R. Thompson, C. W. White

Studies of fluxoid lattice arrays, flux flow, flux creep, fluxoid defect interactions, and anisotropy in Nb-, V-, and Ta-base alloys and superconducting compounds with A15 and B1 crystal structures; small-angle neutron scattering by equilibrium and metastable fluxoid lattice configurations in superconductors; dc magnetization, ac magnetic permeability, critical-current and normal-state electrical transport; ion damage, ion implantation, and ion backscattering in bulk and thin-film superconductors; laser annealing studies of superconductors.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

183. PREPARATION AND CHARACTERIZATION OF RESEARCH MATERIALS — $630,000 — 02-2

L. A. Boatner, W. E. Brundage, Y. K. Chang, L. S. Darken, G. R. Gruzalski

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 ($K_{1-x}Li_xTaO_3$, $KTaO_3$, $KTa_{1-x}Nb_xO_3$) and semiconducting oxides for photoelectrochemical cell electrode investigations; float-zone and tri-arc growth of crystals of A15 compounds such as V_3Si, V_3Ge, Ti_3Au, 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.

184. PHOTOPHYSICAL PROCESSES OF SOLAR ENERGY CONVERSION — $735,000 — 02-2

R. F. Wood, J. W. Cleland, L. S. Darken, R. B. James, G. E. Jellison, B. C. Larson, D. H. Lowndes, J. Narayan, G. van der Leeden, R. D. Westbrook, C. W. White, R. T. Young

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.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

185. FUNDAMENTAL ASPECTS OF METAL FRACTURE — $385,000 — 02-2
S. M. Ohr, S.-J. Chang, J. A. Horton, J. Narayan, T. S. Noggle

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.

186. SCATTERING OF SYNCHROTRON RADIATION — $120,000 — 02-2
B. C. Larson, J. F. Barhorst, R. M. Nicklow, T. S. Noggle, C. W. White

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.

187. THEORY OF CONDENSED MATTER — $1,110,000 — 02-3
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

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; lattice vibrations in disordered alloys; coherent potential approximation; vibrational properties around substitutional impurities in insulators; neutron scattering from 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.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

188. X-RAY DIFFRACTION AND ELECTRON MICROSCOPY — $680,000 — 02-4
B. C. Larson, J. F. Barhorst, J. Narayan, T. S. Noggle, S. M. Ohr, S. Pennycook, J. A. Horton

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 Cu, Ni, Au, Ag, Si, Nb, and stainless steel; 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; solid phase recrystallization in semiconductors; 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.

189. GASES IN METALS — $240,000 — 02-4
D. B. Poker, J. M. Williams, R. R. Coltman, C. E. Klabunde

Interactions of light gas atoms with defects in metals; diffusivity of ion-implanted He in Ni, Cu, and stainless steels at low temperatures; lattice distortion and diffusivity of H in Mg; techniques include internal friction, ion implantation, mass spectrometry, and thermal desorption spectroscopy.

190. SURFACE PHYSICS AND CATALYSIS — $775,000 — 02-5
L. H. Jenkins, H. L. Davis, J. R. Noonan, G.-C. Wang, J. F. Wendelken, C. W. White, D. M. Zehner

Studies of crystallographic and electronic structure of clean and adsorbate-covered metal and semiconductor surfaces with emphasis on surfaces which either reorder 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), 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.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

191. ION BEAM ANALYSIS AND ION IMPLANTATION $925,000 02-5
B. R. Appleton, J. H. Barrett,
G. M. Beardsley, Y. K. Chang,
R. J. Culbertson, O. W. Holland,
E. J. Kelly, C. J. McHargue,
H. Naramoto, J. Narayan,
T. S. Noggle, O. E. Schow III,
B. W. Stritzker, C. W. White,
J. M. Williams, S. P. Withrow

Continued development of positive ion crystallography of surfaces (PICS) technique; application of PICS to reordered and relaxed metal surfaces and to metastable semiconductor surfaces formed by pulsed-laser annealing; fundamental studies of laser annealing; studies of high-speed nonequilibrium crystal growth; investigations of segregation, constitutional supercooling, substitutionality, and solute trapping effects; determination of mechanisms limiting maximum substitutional concentrations of ion-implanted impurities subjected to pulsed-laser processing; study of supersaturated substitutional alloys, new metastable phases and amorphous alloys fabricated by ion beam and pulsed-laser processing; fundamental investigations of ion beam and laser-induced materials interactions; 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 of wear, hardness, and structural properties of ceramics, to improvements in high-temperature materials, and to the fabrication of high transition temperature superconductor compounds from thin film composites; fundamental studies of ion-solid interactions (particularly ion channeling) with applications to materials analyses.

192. RADIOACTIVE WASTE STORAGE $420,000 02-5
L. A. Boatner, M. M. Abraham,
S. C. Corbato, M. Petek,
B. C. Sales

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 and of phases present in other nuclear waste forms (e.g., perovskite $CaTiO_3$, zircon $ZrSiO_4$); 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 and other surface analytical techniques.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

193. RESEARCH AND DEVELOPMENT - ISOTOPE RESEARCH MATERIALS PREPARATION — $300,000 — 02-5
E. H. Kobisk, W. S. Aaron, H. L. Adair, T. C. Quinby, R. D. Taylor

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, isostatic 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
P. O. Box X
Oak Ridge, Tennessee 37830

Chemistry Division -03-
O. L. Keller - Phone: (FTS) 624-4987 or 615-574-4987

194. CHEMICAL STRUCTURE OF ENERGY RELATED MATERIALS — $970,000 — 03-1
W. R. Busing, G. M. Brown, E. Johnson, A. H. Narten, W. E. Thiessen

Atomic and molecular arrangements in crystals and in liquids determined by neutron and x-ray diffraction studies; atom-atom pair correlation functions for liquids; particle size distribution function in 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; modeling of phase changes in crystals. Materials studied include solid coal and its liquid extracts, 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 solutions, and glasses used for optical communications.

195. HIGH TEMPERATURE CHEMISTRY AND THERMODYNAMICS OF STRUCTURAL MATERIALS — $620,000 — 03-2
C. E. Bamberger, J. Brynestad, G. M. Begun, C. E. Vallet

High temperature materials of importance scientifically and technically are synthesized and characterized by new approaches: for example, titanium diboride, TiB_2, is being synthesized by homogeneous nucleation from several gaseous phases under various controlled conditions and commercial products are being purified by reaction with gaseous BCl_3. Studies have been completed of selected microphases in high temperature steels. The stabilities and structures of carbides, Fe-Cr binaries, and other microphases were determined by x-ray diffraction using synchrotron radiation and other applicable techniques; also, studies have been completed of synthetic monazites and monazite-type solid solutions of potential interest in nuclear waste immobilization. coprecipitation of Bi(III) and Ce(IV) by phosphate yielded, after ignition, monazite-type solid solutions identifiable by Raman spectroscopy.

OAK RIDGE NATIONAL LABORATORY
Chemistry Division -03- (continued)

196. LOCALIZED CORROSION AND STRESS CRACKING PHENOMENA RELATED TO ENERGY TECHNOLOGIES — $680,000 — 03-3
F. A. Posey, A. L. Bacarella, H. R. Bronstein, G. M. Brown, E. J. Kelley, A. A. Palko

Application of electrochemical methods coupled with ion implantation/Rutherford backscattering techniques to basic studies of mechanisms of aqueous corrosion reactions occurring in localized attack of metals (titanium, vanadium, 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; use of electrochemical methods in development of processes for treatment of photographic and photoreproduction effluents for detoxification and silver recovery.

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

Chemical Technology Division -03-
D. E. Ferguson - Phone: (FTS) 624-6148 or 615-574-6148

197. CHEMICAL ENGINEERING RESEARCH — $235,000 — 03-2
D. F. Williams, C. H. Byers

Fundamental measurement and theoretical framework for materials properties of liquid mixtures at extreme conditions; development of laser light scattering techniques for properties measurements of organic mixtures such as model coal conversion streams. Viscosities, diffusion coefficients and interfacial properties at high pressures and temperatures. Property correlation and development of predictive relationships. Submicron filtration of gases in deep granular beds under electrostatic enhancement.

198. THERMODYNAMICS OF ENERGY RELATED SYSTEMS — $252,000 — 03-2
T. B. Lindemer, E. C. Beahm, T. M. Besmann

Fundamental experimental and theoretical chemical thermodynamics studies, usually associated with oxide and carbide breeder reactor fuels. Phase equilibria and thermodynamic properties of the systems Pu-O and U-Pu-O, $U(C,O)_{1.9}$-U(C,O); $PuO_{1.5}$-$PuC_{1.5}$-Pu(C,O); $PuO_{1.5}$-$PuC_{1.5}$-C; (U,Pu)(C,O)-$(U,Pu)C_{1.5}$; and $(U,Pu)O_2$-$(U,Pu)C_{1.5}$-C. Basic chemical compatibility of uranium carbides with Cr-Fe-Ni alloys. Thermodynamics properties and compounds in the systems U-Pu-C-Cr-Fe-Ni and U-Pu-C-Ni.

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

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

199. DEGRADATION OF CERAMICS IN COAL DERIVED ENVIRONMENTS — $74,000 — 01-1
J. L. Bates

The mechanisms and kinetics of high temperature reactions of refractory metal oxides with molten silicates and gases representative of coal derived systems; 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; initial studies react $MgAl_2O_4$, MgO or Al_2O_3 with liquid $CaO-Al_2O_3-SiO_2$ containing iron and magnesium.

200. PHOTOELECTROCHEMICAL PROPERTIES OF SOLAR MATERIALS — $87,000 — 01-1
R. Wang

Effects of crystal structure, microstructure and composition on the photoelectrochemical behavior of semiconductors and semiconducting films in liquid electrolytes. Study the anodic dissolution of metal oxides, formation and properties of anodic films on amorphous alloy surfaces; degradation and corrosion of photoelectrodes; and surface modification for enhanced stability and efficiency.

201. SPUTTER-DEPOSITED AMORPHOUS SILICON FOR SOLAR APPLICATIONS — $82,000 — 01-1
P. M. Martin and W. T. Pawlewicz

Influence of H content and Si-H bonding on optical and electrical properties of sputter-deposited Si:H alloys; Si-H reaction kinetics and film-plasma interaction during film growth; applications to photovoltaic solar cells, thin film coatings and multilayer dielectric stacks; optical and IR spectroscopic techniques, electrical transport measurements, gas evolution analysis; photoconductivity, x-ray fluorescence and x-ray diffraction.

PACIFIC NORTHWEST LABORATORY (continued)

202. EFFECT OF COAL MICROSTRUCTURE ON PROPERTIES — $82,000 — 01-1
J. M. Lytle and J. L. Daniel

Quantitative characterization of coal properties including mechanical, fracture, microstructural, compositional, and thermal; determination of the effect of particle size on these properties (i.e., open and closed porosity, gas evolution, surface area, shapes of particles and strength) and characterization of newly-formed surfaces during coal comminution under controlled temperature and atmosphere conditions; correlation of particle properties with bulk properties; determination of the modes and mechanisms of fracture during coal comminution and the interrelationships between coal properties and fracture modes and mechanisms.

203. FUNDAMENTAL STUDIES OF STRESS CORROSION AND CORROSION FATIGUE MECHANISMS — $230,000 — 01-2
R. H. Jones, M. T. Thomas, S. M. Bruemmer, D. R. Baer and M. J. Danielson

Investigations of the mechanisms controlling intergranular and transgranular stress corrosion and corrosion fatigue cracking of iron, iron-chromium-nickel and nickel-based alloys in gaseous and aqueous environments. 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.

204. OXIDATION AND CORROSION RESISTANT FINE-GRAINED MATERIALS — $105,000 — 01-3
J. T. Prater and D. R. Baer

Investigate the mechanisms controlling the high-temperature corrosion of sputtered-deposited fine-grained materials. Oxidation and sulfidation studies of stainless steel in CO-CO_2 and CO-CO_2-H_2S gaseous environments at 800 to 1000°C, and hot corrosion studies on $Fe_{39}Co_{27}Cr_{22}Al_9Ni_3Y_1$ covered with Na_2SO_4 in an SO_2-O_2 atmosphere at 650 to 800°C. Use SEM, STEM, microfocus x-ray diffraction and mechanical tests to determine the effect alloy grain size, alloying additions, and gaseous environment have on scale microstructure, scale adherence and scale cracking behavior. Employ AES, XPS, and nuclear microprobe measurements to examine the diffusion and bonding state of elements at the alloy surface as the corrosion process proceeds.

PACIFIC NORTHWEST LABORATORY (continued)

205. LEACHING OF GLASS AND CERAMICS $95,000 01-3
G. L. McVay and L. R. Pederson

Mechanistic investigations of glass and crystalline ceramic interactions with aqueous solutions. Primary emphasis is upon the elemental interactions in the reaction layer (region between unaffected bulk material and the solution). Research areas include: surface potential measurements, radioactive tracer diffusion measurements, isotopic water reactions coupled with Rutherford backscattering and nuclear microprobe analyses, resorption kinetics, solution analyses, pH and oxygen level effects, and surface and near-surface analyses using primarily Raman, ESCA and SIMS coupled with ion milling. Major goal is development of a predictive model for leaching.

206. RADIATION EFFECTS IN METALS AND CERAMICS $620,000 01-4
E. P. Simonen, J. L. Brimhall,
G. J. Exarhos, E. R. Bradley,
L. A. Charlot, C. H. Henager, Jr.,
H. E. Kissinger and W. J. Weber

Evaluation of radiation damage mechanisms in metals and non-metals; irradiation of metals using heavy-ion, light-ion, neutron and electron 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; pulsed irradiation effects on creep and microstructures; effects of primary damage on amorphous and crystalline phase stability; studies of nickel, molybdenum, ferritics, amorphous metals, ordered intermetallic compounds. Studies of damage in stoichiometric non-metals using external alpha bombardment or internal alpha-recoil particles; characterization and modeling of the state and kinetics of damage in-growth and annealing utilizing x-ray diffraction, electron microscopy, density measurements, optical absorption and vibrational Raman scattering; ionization damage; studies of cubic oxides and fluorides, amorphization of rare earth silicates and phosphates.

207. SPUTTERING PARAMETER INFLUENCES ON MATERIAL STRUCTURE AND BEHAVIOR $200,000 01-5
E. D. McClanahan, W. T. Pawlewicz
and R. W. Knoll

Research on the process of high-rate sputtering to permit characterization and definition of the influence of sputtering parameters on the structure and behavior of sputter-deposited metallic and insulator materials. Study areas for metals (Mo and rare earth-transition metal alloys) include investigation and modeling of the parameters which influence the incorporation of gases (Kr, H_2 and CO) during sputter deposition, and investigation of relationships between structure, properties and thermal stability of metals containing significant quantities of gases. Study areas for insulators (ZrO_2) include stoichiometry, structure, properties, adherence to metallic substrates and controlled deposition at high rates. Materials characterization includes x-ray fluorescence and diffraction, matallography, SEM, TEM, thermal gas evolution analysis, electrical and optical property measurement, gas chromatography, calorimetry and differential thermal analysis. Particle energy and mass are analyzed during deposition.

PACIFIC NORTHWEST LABORATORY (continued)

208. OPTICAL AND LASER MATERIAL STUDY — $120,000 — 02-2
J. S. Hartman, J. W. Griffin, L. S. Dake, M. A. Lind and L. R. Pederson

Research on adhesion mechanisms at the silver/substrate interface in second surface mirrors before and after exposure to terrestrial environmental stresses (temperature, humidity, UV radiation): preparation and evaluation of mirrors as a function of (1) substrate material (simple crystalline: quartz; amorphous: fused silica; and complex: soda-lime silicate glass); (2) substrate preparation (abrasion, chemical cleaning, sputter etch); and (3) silver deposition techniques (wet chemistry, e-beam, rf sputtering); sample evaluation to include ellipsometry, photo-acoustic spectroscopy, adhesion testing, optical properties (spectral reflectivity and scattering), chemical properties of interface region (AES, SIMS, and ESCA) sample morphology (SEM and optical microscopy), x-ray diffraction, Raman spectroscopy.

209. SPUTTER-DEPOSITED COATINGS FOR OPTICAL APPLICATIONS — $120,000 — 02-2
W. T. Pawlewicz, P. M. Martin and D. D. Hays

Study of the optical properties of dielectric materials in thin-film form. Oxides, nitrides and elemental semiconductors are presently investigated. Measurement, modeling and understanding of relationships between optical properties and materials properties. Control of materials properties through understanding of the reactive sputtering process. Optical properties include the spectral dependence of the complex refractive index; fundamental interband and lattice vibration absorption edges; scattering; optical homogeneity, uniformity and isotropy. Materials properties include structure, microstructure, bonding in amorphous materials, stoichiometry, composition, purity and surface topography. Measurement techniques include transmission and reflection spectrophotometry, x-ray diffraction, STEM, x-ray flourescent analysis, Nomarski microscopy and XPS.

210. NANOMETER MACHINING AND GRINDING DEVELOPMENT — $60,000 — 02-5
N. Laegreid and D. M. Miller

Utilize unique Omega-X Machine Tool to develop machining technology permitting achievement of surface roughness less than 1.5 nanometer rms, and total contour accuracy of 100 nanometer for flat, concave, and convex spherical and aspherical surfaces up to one meter diameter. Identification and problem solving applied to machine tool, cutting tool, materials and part geometry limitations.

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

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

211. STRESS CORROSION CRACKING AND ELECTROCHEMISTRY OF TRANSIENT CORROSION PROCESSES — $185,000 — 01-2

W. H. Smyrl
R. J. Salzbrenner

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.

212. ION IMPLANTATION AND DEFECTS IN MATERIALS — $635,000 — 01-3

P. S. Peercy
K. L. Brower
B. L. Doyle
H. J. Stein
D. M. Follstaedt
J. A. Knapp
S. M. Myers
S. T. Picraux

Modification and analysis of near surface regions of solids are being studied using ion beam techniques. Ion implantation metallurgy is used to determine phase diagrams, diffusion coefficients and solubilities, and to investigate the trapping, transport and surface recombination of hydrogen in Fe and Ni and in Fe-based alloys. Ion implantation, ion beam mixing, laser and electron beam annealing are used to form equilibrium and nonequilibrium alloys which are then studied using ion beam analysis and electron microscopy techniques. New techniques are being developed to study dynamic parameters, such as melt depth, melt velocity and regrowth velocity during laser annealing. Corrosion, diffusion, and electrical behavior are studied in amorphous surface layers formed by ion implantation in metals and semiconductors. Ion beam techniques are used to control disorder and H in amorphous silicon to permit investigation of the fundamental structure and defect properties. Defects and metastable solutions in ion implanted and laser-annealed semiconductors are studied using EPR and optical techniques.

SANDIA NATIONAL LABORATORIES-Albuquerque (continued)

213. EROSION AND WEAR — $240,000 — 01-5
R. E. Cuthrell
T. A. Mechalske
J. J. Mecholsky

This task addresses the subject of erosion and wear by studying the individual fracture and fatigue mechanisms that collectively contribute to the wear process. Specifically, chemical-mechanical synergistic effects on fracture, crack growth and fatigue are being investigated. The research on wear supports the development of improved testing procedures and guides the development of improved materials and coatings. Experiments on the fracture of brittle materials in high vacuum, pure H_2 and H_2O vapor plus mixtures of H_2 and H_2O have revealed very complex but reproducible effects on fracture strength. Time dependent increases followed by decreases in strength are observed. By controlling the environment, improved consistency in fracture strength of ceramics has been obtained. This reduction in data scatter allows more detailed models to be developed for fracture and wear resistant materials.

214. SEMICONDUCTORS FOR USE AT HIGH TEMPERATURES — $230,000 — 01-5
R. M. Biefeld
L. R. Dawson
I. J. Fritz
P. L. Gourley
G. C. Osbourn

Experimental and theoretical studies of bulk and interfacial high temperature properties of wide bandgap semiconductors ($Eg \geq 1.4$ eV). Objective is identification of candidate materials and contact metallizations suitable for high temperature (to 500°C) active semiconductor devices. The work has a comprehensive fundamental scope, incorporates modern materials growth techniques (including liquid phase epitaxy, molecular beam epitaxy and metal-organic chemical vapor deposition) and is coordinated with device physics programs to give this research technological impact. Studies include doping, transport, optical and defect properties. Current emphasis has been on GaP, GaP-based materials and GaAlAs.

SANDIA NATIONAL LABORATORIES-Albuquerque (continued)

215. ELECTRON AND PHOTON-STIMULATED DESORPTION — $230,000 — 02-2

M. L. Knotek, G. M. Loubriel, D. R. Jennison, R. H. Stulen

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 are being carried out using Electron- and Photon-Stimulated desorption techniques (ESD and PSD). These investigations exploit the discovery that desorption occurs by Auger decay of radiation induced core holes. This allows the extraction of site specific, adsorbate specific electronic and structural information since both the local empty density of states and extended x-ray absorption fine structures are sampled. These techniques are uniquely surface sensitive and sample only the uppermost layer of surface atoms. The high sensitivity to hydrogen will be exploited in the study of its role in catalysis, corrosion and semiconductor technology.

216. STUDIES OF THE VAPOR PHASE OF THE CHEMICAL-VAPOR-DEPOSITION PROCESS — $200,000 — 02-2

A. W. Johnson, W. G. Breiland, G. C. Tisone, M. E. Coltrin

Studies of important vapor-phase reactions and nucleation processes during CVD deposition of photovoltaic cells, corrosion-resistant coatings, and semiconductor materials. 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. Development of a predictive model including 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.

217. STABILITY AND CHARGE-TRANSFER PROPERTIES OF THE SOLID-LIQUID INTERFACE — $100,000 — 02-2

M. A. Butler, D. S. Ginley

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 surfaces 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.

SANDIA NATIONAL LABORATORIES-Albuquerque (continued)

218. SURFACE PHYSICS RESEARCH $280,000 02-2

M. L. Knotek D. R. Jennison
J. E. Houston R. R. Rye
J. A. Panitz G. L. Kellogg

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

SANDIA NATIONAL LABORATORIES
Livermore, California 94550

B. F. Murphey - Phone (FTS) 532-2884 or (415) 422-2884
Walter Bauer - Phone (FTS) 532-2994 or (415) 422-2994

219. GASES IN METALS $210,000 01-2
W. D. Wilson (FTS) 532-2884 or (415) 422-2664
G. J. Thomas
M. I. Baskes

This is a coupled experimental and theoretical program aimed at understanding the behavior of helium, hydrogen and other gaseous impurities in metals and their influence of mechanical properties. Quantum theoretical calculations have predicted the formation of embryonic helium bubbles and associated self-interstitials in the absence of radiation damage. The experimental techniques of electron microscopy, electron energy loss spectroscopy, small angle neutron scattering and thermal desorption spectroscopy have been applied to study helium clustering phenomena in sub-damage-threshold implanted gold and in tritiated metals. Measurements of hydrogen diffusion, trapping and partial molal volume have been made in nickel and stainless steel using laser interferometry, desorption and tritium autoradiography. Theoretical calculations of the chemical and physical binding of hydrogen to impurities in metals have been performed.

220. PROTECTIVE BARRIERS AND COATINGS FOR COMBUSTION MATERIALS $290,000 01-1
R. E. Palmer (FTS) 532-3126 or (415) 422-3126
R. E. Benner
A. S. Nagelberg
J. C. Hamilton

A program to study corrosion/erosion mechanisms in high temperature environments utilizing optical diagnostic methods to observe the attack process. A Materials Research Combustion Simulator is being used for erosion studies at elevated temperatures. Mechanisms of hot corrosion by molten salt deposits are under investigation using a high temperature furnace with wide angle optical access for in-situ Raman analysis. Corrosion by mixed gas phase oxidants will receive increasing emphasis. In-situ observations will be supplemented by appropriate post exposure analysis.

221. DIAGNOSTICS FOR COMBUSTION MATERIALS RESEARCH $110,000 02-5
R. E. Palmer (FTS) 532-3126 or (415) 422-3126
R. E. Benner
R. L. Farrow
J. C. F. Wang

A program aimed at the development of laser-based diagnostic techniques to study corrosive/erosive processes at high temperatures. A Materials Research Combustion Simulator, a facility available to outside users for simulating relevant combustion environments, has been equipped for high temperature Raman scattering studies of corrosion/erosion and oxidation of materials and coatings for use in advanced turbines. Optical diagnostic methods are available to characterize the simulated environments and to monitor surface processes during exposure. Complementary post-exposure techniques are used to supplement the optical diagnostics.

SOLAR ENERGY RESEARCH INSTITUTE
1617 Cole Boulevard
Golden, Colorado 80401

Solar Thermal and Materials Research Division - Materials Research Branch
G. E. Gross - Phone: (FTS) 327-1228 or (303)231-1228; or
S. Bull - Phone: (FTS) 327-7723 or (303)231-7723

222. SOLAR MATERIALS RESEARCH $290,000 01-1
A. W. Czanderna, P. Schissel, J. Webb,
J. R. Pitts, T. Thomas

Mechanisms of materials degradation affecting the performance in solar energy conversion systems; interface studies in the glass/silver, silica/silver, silver/copper 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 polymethymethacrylate; 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.

SECTION B

Contract Research

(Primarily Universities)

This information was prepared by the DOE project monitor. 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 — $ 98,155 (13 months) — 02-2
J. M. Cowley - Dept. of Physics
Phone: (602)-965-6459

High resolution scanning transmission electron microscope study of surface reaction products by electron microdiffraction and selective imaging. In particular, a study of the crystal structure, morphology and epitaxial relationships of oxide microcrystals formed on chromium thin films and iron-chromium alloys. Also, parallel studies on the oxidation of bulk crystals by the methods of reflection electron diffraction, scanning electron microscopy and dark-field scanning microscopy on pyrolytic graphite.

302. TRANSPORT IN SOLID ELECTROLYTES CONTAINING A DISPERSED SECOND PHASE — $ 67,349 (10 months) — 01-3
J. B. Wagner, Jr. - Center for Solid State Science
Phone: (602)-965-6959, 4544

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 SiO_2, 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.

BATTELLE COLUMBUS LABORATORIES

303. FAILURE OF CERAMICS FROM MULTIAXIAL STRESSES — $142,000 — 01-5
A. R. Rosenfield, D. K. Shetty,
S. G. Sampath, W. H. Duckworth
Phone: (614)-424-4353

Understanding of multiaxial stress phenomena on the mechanical behavior of ceramics. 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. Materials preparation and characterization. Fractography. Three dimensional linear elastic finite element analysis of test-specimen geometries and for stress-intensity factors. Biaxial tests of ceramic specimens containing controlled artificial flaws. Al_2O_3, SiC, Si_3N_4, glass-ceramics.

BOSTON UNIVERSITY

304. INFRARED ABSORPTION SPECTRUM OF FREE CARRIERS IN POLAR SEMICONDUCTORS: OPTICAL ABSORPTION AND ELECTRON TRANSPORT AT HIGH FIELDS IN BULK AND LAYERED COMPOUNDS — $ 70,730 — 02-3

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

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.

BROWN UNIVERSITY

305. A COMBINED MACROSCOPIC AND MICROSCOPIC APPROACH TO THE FRACTURE OF METALS — $201,000 — 01-2

R. J. Asaro - Division of Engineering
Phone: (401)-863-1456
J. Gurland - Division of Engineering
Phone: (401)-863-2628
A. Needleman - Division of Engineering
Phone: (401)-863-2863

Analysis and measurement of fracture in metals, principally steels; stable crack growth models for elastic-ideally plastic materials under small scale yielding conditions; application of models to high strength steels; cavitation as a function of plastic strain, particle size, stress triaxiality and H_2 activity during ductile fracture of plain carbon steels; creep cavity growth in deformation vs diffusion controlled regimes under multiaxial loading; validity of singularity describing crack tip strain fields during load transients.

306. TIME RESOLVED FAR INFRARED SPECTROSCOPY OF EXCITONS — $ 59,000 — 02-2

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

High-resolution, time-resolved spectroscopy of excitons in semiconductors at far IR wavelengths with subnanosecond speed. Will use tunable submillimeter wave laser to study III-V and II-VI semiconductors.

CALIFORNIA INSTITUTE OF TECHNOLOGY

307. MELTING IN ADSORBED FILMS $ 74,663 02-2
D. Goodstein - Dept. of Physics
Phone: (213)-356-4315

Study of two-dimensional melting of methane on Grafoil and how two-dimensional melting is related to three-dimensional melting. Systematic thermodynamic measurements will be made in the temperature range 2-100 K with coverages of 0-5 monolayers. Dynamic studies will be made using pulsed NMR.

308. STUDIES OF ALLOY STRUCTURE AND PROPERTIES $204,977 01-1
W. L. Johnson - Division of Engineering and Applied Science
Phone: (213)-356-4433

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.

309. THE PRESSURE DEPENDENCE OF THE MECHANICAL PROPERTIES OF POLYMERS $ 36,300 01-2
N. W. Tschoegl - Dept. of Chemistry & Chemical Engineering
Phone: (213)-356-4676

Development of constitutive equations describing the time-temperature-pressure effects on shear relaxation in elastomers, specifically rubber with various crosslink densities; determination of compressibility and thermal expansion up to 10 kbars; time-dependent Poisson ratio measurement; analysis of behavior near glass transition temperature.

UNIVERSITY OF CALIFORNIA/DAVIS

310. RADIATION DAMAGE AND ENVIRONMENT EFFECTS IN NUCLEAR WASTE STORAGE MEDIA — $ 72,000 (10 months) — 01-1

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

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.

311. DEFORMATION MECHANISMS AND FAILURE MODES IN SUPERPLASTICITY — $ 72,000 (14 months) — 01-2

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

Experimental and analytical study of superplastic deformation of metals, specifically Zn-Al, Ni-base, 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 as well as independent and parallel creep mechanisms in alloys after various thermomechanical processing; relationship of above to superplastic forming.

312. AN INVESTIGATION OF THE ROLE OF SINTERING IN GAS-SOLID INTERACTIONS — $ 66,572 (13 months) — 01-3

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

Investigation of the role of sintering in the kinetics of gas-solid interactions in powder compacts, including both oxidation-reduction and dissociation reactions. 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. Materials systems under investigation include Pd/PdO, Fe/FeO, and dissociation reactions of carbonates and hydroxides.

UNIVERSITY OF CALIFORNIA/IRVINE

313. RAMAN SPECTROSCOPY OF MOLECULAR ADSORBATES — $106,000 — 02-2

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

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.

314. INTERACTION OF LOW ENERGY ELECTRONS WITH SURFACE LATTICE VIBRATIONS — $ 86,569 — 02-2

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

Theory of inelastic scattering of electrons by vibrating atoms and molecules at solid surfaces. Role of image potential in electron energy-loss spectroscopy (EELS) with low impact energies. Applications to H on W, and NH_3 and CO on Ni, Pt, Rh, and Ir. Theory of lattice dynamics of clean and adsorbate-covered surfaces and of thermal diffuse scattering of electrons from clean transition metal surfaces. This program is strongly coupled with that of S. Y. Tong, University of Wisconsin - Milwaukee.

UNIVERSITY OF CALIFORNIA/LOS ANGELES

315. IRRADIATION-INDUCED PRECIPITATION AND SOLUTE SEGREGATION IN ALLOYS — $ 90,482 — 01-4

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

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

316. INVESTIGATION OF THE INTERACTION BETWEEN SUPERCONDUCTIVITY AND MAGNETISM AND OSCILLATORY CHEMICAL REACTIONS OVER METAL SURFACES — $252,000 (13 months) — 02-2

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

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 new rare earth compounds such as $ErRh_4B_4$ and $ErMo_6Se_8$ will be studied in order to understand re-entrant and coexistence phenomena. A new effort in surface physics has been started with a study of the oscillatory oxidation of CO on Pt and a study of some metallic thin film oxidations.

317. RESEARCH ON THE THERMOPHYSICAL PROPERTIES OF MATERIALS — $126,663 — 02-5

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

Studies of the science of heat engines and the materials which work in them. The following specific areas are included: (1) Heat engines (Stirling-Malone and Brayton cycles) using liquid working substance and their possible application to the heating and cooling of structures, (2) Basic thermal and mechanical principles of a prime mover (Stirling-Malone cycle) using liquid water as working substance, (3) Fundamental reexamination of heat engine science using cryogenic temperatures and the helium isotopes as working substances, (4) Gravitational convection of energy in dilute solutions of ^3He in superfluid ^4He as a model of convective processes in a low Prandtl number insulating fluid where stochastic processes are known to be important, (5) Search for a quasi-particle-driven instability in ^3He-^4He solutions near the tricritical point, (6) Preliminary experimental considerations on the study at low temperatures of both the "electron in vacuum" and the "electron bubble in superfluid ^4He" non-neutral plasmas.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA

318. RESONANCE STUDIES OF SUPERIONIC CONDUCTORS — $ 77,000 — 02-2

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

NMR and EPR study of superionic and related compounds. Computer simulation of ion hopping processes. Low frequency measurements on $Mn:PbF_2$ and $H:PbF_2$ to determine importance of H^- diffusion and its relation to F^- mobility in ionic conduction. Determine charge states of Fe in $Co^{57}:PbF_2$ by Mössbauer studies.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA (continued)

319. RESEARCH ON PHASE TRANSFORMATIONS AND NON-EQUILIBRIUM PROCESSES — $ 84,542 — 02-3
J. S. Langer - Dept. of Physics
Phone: (805)-961-3495

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 multi-component fluids.

CARNEGIE INSTITUTION OF WASHINGTON

320. STUDY OF THE PROPERTIES OF HYDROGEN AT STATIC PRESSURES OF ONE MEGABAR — $100,000 — 02-2
P. M. Bell - Geophysical Laboratory
Phone: (202)-966-0334
H. K. Mao - Geophysical Laboratory
Phone: (202)-966-0334

Investigations of hydrogen under very high pressure. Hydrogen was pressurized to 900 Kbar, and a static pressure of 650 Kbar was achieved. Laser Raman scattering of molecular bonding phenomena as a function of pressure in hydrogen and deuterium. Brillouin scattering measurements of hydrogen up to 250 Kbar. Single crystals of neon examined up to 250 Kbar. X-ray pressure cell development.

CARNEGIE-MELLON UNIVERSITY

321. FUNDAMENTAL STUDIES OF EROSION AND EROSION/CORROSION FOR COAL GASIFICATION SYSTEMS — $ 64,099 — 01-5
J. C. Williams - Dept. of Metallurgy and Materials Science
Phone: (412)-578-2704
G. B. Sinclair - Dept. of Mechanical Engineering
Phone: (412)-578-2504

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-Co and Cu-Ni alloys, steels; techniques - laser interferometry, electron microscopy.

CASE WESTERN RESERVE UNIVERSITY

322. COUPLED DIFFUSION PHENOMENA IN MULTICOMPONENT GLASSES AND GLASS FORMING LIQUIDS — $ 83,000 — 01-3

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

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.

323. MICROSTRUCTURAL DEVELOPMENT IN OXIDE CERAMICS — $ 90,000 — 01-2

A. H. Heuer - Dept. of Metallurgy and Materials Science
Phone: (216)-368-4224

Effect of non-stoichiometry on plastic deformation in UO_{2+x}. Microstructural stability and evolution in Al_2O_3-ZrO_2 toughened composites.

324. EXPERIMENTS IN HIGH VOLTAGE AND ANALYTICAL ELECTRON MICROSCOPY — $ 95,000 (13 months) — 01-4

T. E. Mitchell - Dept. of Metallurgy and Materials Science
Phone: (216)-368-4210

Study of irradiation damage in metals and ceramics by high voltage electron microscopy with supplementary experiments using ion and neutron irradiation for comparison purposes. Studies of irradiation effects on alloys include defect clustering, phase stability, segregation and order-disorder phenomena, particularly in β phase alloys such as FeAl and NiAl. Studies of irradiation effects on ceramics include amorphization by ionization damage in SiO_2 and GeO_2 polymorphs and various silicates, displacement damage leading to the growth of defect clusters in simple oxides such as MgO, NiO, and BeO, void growth in oxides susceptible to swelling such as Al_2O_3, and phase decomposition and defect stabilization in more complex swelling-resistant ceramics such as spinel, YAG, and Si ceramics.

UNIVERSITY OF CHICAGO

325. RESEARCH IN THE THEORY OF CONDENSED MATTER AND ELEMENTARY PARTICLES — $125,350 — 02-3

L. P. Kadanoff - The James Franck Institute
Phone: (312)-753-8205
Y. Nambu - The James Franck Institute
Phone: (312)-753-8608

The research aims to elucidate problems which are apparently relevant to both elementary particle physics, through quantum field theory, and condensed matter physics--via the statistical mechanics of phase transitions. String theories and problems in two-dimensions of space (or one of space and one of time) will get considerable attention. Topics under consideration will include Hamiltonian and equation of motion methods for approaching string theory, multicritical points and bifurcation theory in two dimensions, parafermion fields, Monte Carlo renormalization group analyses, and studies of the stability of gauge theories under small perturbations.

COLORADO SCHOOL OF MINES

277,000

326. FERROUS ALLOY METALLURGY - LIQUID LITHIUM CORROSION AND WELDING — $145,000 — 01-5

D. Olson - Dept. of Metallurgical Engineering
Phone: (303)-279-0300, x787
D. Matlock - Dept. of Metallurgical Engineering
Phone: (303)-279-0300, x775

Dissolution kinetics of austenitic stainless steels in molten Li; corrosion fatigue and embrittlement of ferritic steels in molten Li; influence of welding parameters on the microstructure and mechanical properties of dissimilar ferrous metal weldments; effect of liquid lithium on the fatigue behavior of 2¼ Cr-1 Mo steel; Auger electron spectroscopy of fracture surfaces; 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.

UNIVERSITY OF COLORADO

327. LIGHT SCATTERING STUDIES OF LOWER DIMENSIONAL COLLOIDAL PARTICLE AND CRITICAL FLUID SYSTEMS — $ 90,000 — 02-2

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

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

328. DEFECT INTERACTIONS AT HIGH CONCENTRATIONS IN SOLID OXIDE ELECTROLYTES — $ 66,643 — 01-3

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

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 and electrical properties; relationship between simple defects that form at low concentrations and the ordering and microdomain formation observed at high concentrations; kinetics of cationic ordering. Electrode phenomena. 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 $Zr_3ER_4O_{12}$. 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

329. ELECTRODE POLARIZATION STUDIES IN HOT CORROSION SYSTEMS — $ 68,000 — 01-3

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

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.

330. ELECTRON-DISLOCATION INTERACTIONS AT LOW TEMPERATURES — $ 12,932 — 01-2

J. M. Galligan - Dept. of Metallurgy
Phone: (203)-486-3541, 4623

Determination, in an ordinary tensile test, of velocity of mobile dislocations, electron-dislocation drag, and mobile dislocation density. Experiments measure change in stress for plastic deformation accompanying change in magnetic field. Effects of crystal orientation. Occurrence of magneto-oscillations in stress field as a function of temperature, magnetic field, and applied strain rate at specific angles relative to principal axes of a crystal.

UNIVERSITY OF CONNECTICUT (continued)

331. ENERGY TRANSFER AND NON-LINEAR OPTICAL PROPERTIES AT NEAR ULTRA-VIOLET WAVELENGTHS: RARE EARTH 4f → 5d TRANSITIONS IN CRYSTALS AND GLASSES — $100,000 — 02-2
D. Hamilton - Dept. of Physics
Phone: (203)-486-3856

Two main areas will be addressed in this program: First the study of energy transfer among the same chemical species of ions in their 5d configuration for crystalline and amorphous host materials, second, the extension to transfer between different species. The primary technique to be employed is dynamic polarization spectroscopy-DPS.

332. THE FATIGUE BEHAVIOR OF 9- AND 12 Cr FERRITIC STEELS AT ELEVATED TEMPERATURE — $ 57,000 — 01-2
A. J. McEvily - Metallurgy Department
Phone: (203)-486-2941

Creep-fatigue behavior of ferritic steels (9-12% Cr) related to micro-structural features (grain size, carbide distribution, bainitic vs martensitic structure), oxidation resistance fracture mechanics parameters, and fabrication (wrought vs welded condition).

333. INVESTIGATION OF ROLE OF SUBSURFACE ZONES IN WEAR OF MATERIALS — $ 82,307 — 01-5
S. Rice - Dept. of Mechanical Engineering
Phone: (203)-486-2153

Experimental characterization of the formation, composition and morphology of 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; for a work hardening elastoplastic material subject to given load cycling and temperature distributions; model development which allows prediction of composition and morphology of subsurface zones for selected materials subjected to both sliding and impulsive contact; and postulation and experimental investigation of in situ development of wear resistance.

CORNELL UNIVERSITY

334. INFLUENCE OF GRAIN BOUNDARIES ON THE ELECTRICAL TRANSPORT PROPERTIES OF POLYCRYSTALLINE SI FILMS — $ 92,500 — 01-1

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

Characterization of the structure and electrical activity of defects in hot pressed and annealed Si bicrystals; examination of Shockley partial dislocations, coherent and asymetric twins, and twist boundaries; passivation of grain boundaries with hydrogenation and thermal treatments; techniques used: HVEM, TEM, electron beam induced charge in SEM.

335. INITIAL STAGES OF OXIDATION OF METALS — $116,200 — 01-1

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

Investigation of the initial stages of oxidation of metals--kinetics, oxide composition and structure, and transition from thin to thick films; detection of Fe_3O_4, FeO, and NiO, and measurement of the ratio of these, during oxidation of $Fe_{40}Ni_{60}$; evaluation of BeO on (0001) Be; techniques used: LEED, AES, TEM, and (planned) synchrotron radiation.

336. MIGRATION OF GRAIN BOUNDARIES IN CERAMIC MATERIALS WITH PARTICULAR REFERENCE TO THE SINTERING PROCESS — $ 81,848 (10 months) — 01-1

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

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 of 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)

337. INELASTIC DEFORMATION IN NON-METALLIC CRYSTALLINE SOLIDS — $ 55,000 — 01-2

D. L. Kohlstedt - Dept. of Materials Science and Engineering
Phone: (607)-256-7144

Liquid-phase hot-pressing and high-temperature deformation of hot-pressed TiC and TiC-VC, and the effects of excess Ti and TiB_2 precipitates on such materials. Densification mechanisms and kinetics. Creep and constant compressive strain rate experiments. TEM-STEM analysis.

338. MECHANICAL PROPERTIES OF CRYSTALLINE SOLIDS — $165,000 — 01-2

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

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.

339. PROBABILISTIC MODELS OF THE STRESS-RUPTURE OF COMPOSITE MATERIALS — $ 76,876 — 01-2

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

Modelling tensile and stress rupture strengths of fiber reinforced polymer composites based on a probabilistic statistics representation of the measured distribution of fiber strengths; 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; influence of fiber strength variation (Weibull modulus) on the importance of matrix properties.

CORNELL UNIVERSITY (continued)

340. HIGH TEMPERATURE MECHANICAL BEHAVIOR OF SILICON NITRIDE — $117,000 (17 months) — 01 2
R. Raj - Dept. of Materials Science and Engineering
Phone: (607)-256-4040

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.

341. DIFFRACTION AND MICROSCOPY STUDIES OF THE STRUCTURE OF GRAIN BOUNDARIES IN Fe, Fe-BASE ALLOYS, AND CERAMIC MATERIALS — $123,000 — 01-1
S. L. Sass - Dept. of Materials Science and Engineering
Phone: (607)-256-5239

Investigation of grain boundary structure in metals, primarily Fe-base alloys, and ceramics--FeO, MgO, NiO, TiC; characterization of boundary periodicity, and dislocation arrays, using TEM imaging as well as electron and X-ray diffraction.

342. DEFECTS IN METAL CRYSTALS — $177,500 — 01-4
D. M. Seidman - Materials Science and Engineering
Phone: (607)-256-2365

Research on the atomic mechanisms undergirding: (a) radiation-induced solute segregation and precipitation in under-saturated binary alloys, (b) radiation-induced formation of metal silicides produced by energetic particle bombardment of metal-silicon sandwiches, (c) radiation-induced segregation of solute atoms to voids and nucleation of voids in fast-neutron irradiated refractory metals and alloys, (d) the formation of metal silicides from metal-silicon sandwiches which have been thermally heated, and (e) the early stages of silicon oxidation. Search for self-interstitial atoms in silicon. Binding of solute atoms to self interstitial atoms and/or to vacancies in metal-silicon alloys. Development of techniques include field-ion microscopy, atom-probe field ion microscopy, conventional transmission electron microscopy, high-voltage electron microscopy (using the DOE Tandem HVEM facility at Argonne National Laboratory), and Rutherford backscattering.

DARTMOUTH COLLEGE

343. THE ROLE OF GRAIN SIZE ON THE BRITTLE TO DUCTILE TRANSITION OF THE STRONGLY ORDERED ALLOY Ni_3Al — $ 76,000 — 01-2

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

Characterization of Ni_3Al powder produced by rapid solidification; consolidation by extrusion; measurement and correlation of grain size with mechanical behavior; use of SEM to evaluate fracture morphology and AES to examine impurity segregation to grain boundaries.

344. SUPERCONDUCTIVITY IN FILAMENTARY EUTECTIC COMPOSITES — $ 54,500 — 02-2

M. P. Zaitlin - Dept. of Physics
Phone: (603)-646-3270

Samples containing niobium filaments in a thorium matrix offer surprising challenges to the understanding of superconducting materials. Measurement of the thermal and electrical conductivity made near the superconducting transition temperature should show coupling between the filaments and between the filaments and the matrix. This coupling is expected to produce a crossover from one-dimensional to three-dimensional superconductivity. Such parameters as filament size, filament spacing as well as matrix composition offer variability in addition to the usual superconductivity measurements.

UNIVERSITY OF DELAWARE

345. ANALYSES OF FAILURE MODES IN SHORT FIBER REINFORCED THERMOPLASTICS — $ 43,900 — 01-2

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

Calculation of physical and mechanical properties of polymers reinforced with discontinuous fibers; thermoelastic constants, thermal conductivity, elastic and shear moduli, and strain hardening found for the parallel fiber case using variational and statistical methods; experimental measurement of elastic constants.

UNIVERSITY OF DELAWARE (continued)

346. RADIATION EFFECTS IN AMORPHOUS METALLIC ALLOYS — $ 80,856 — 02-2

R. B. Murray - Dept. of Physics
Phone: (302)-738-2147
D. G. Onn - Dept. of Physics
Phone: (302)-738-2661
J. J. Kramer - Dept. of Electrical Engineering
Phone: (302)-738-8170

The effects of irradiation on the magnetic and electrical properties of amorphous ferromagnetic Fe-Ni-P-B alloys will be investigated. Complementary resistivity, susceptibility, domain dynamics, electron microscopy, and RHEED studies of irradiated, unirradiated and annealed samples will be used to gain a microscopic structural interpretation for the effects observed.

UNIVERSITY OF DENVER

347. THE DETECTION OF HYDROGEN ASSISTED CRACK GROWTH — $ 74,100 (15 months) — 01-5

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

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 — $ 77,000 — 01-3

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

Effect of solid solutions of various sized ions in cordierite on thermal expansion. Solutes considered are Ge, B, and P substituted on tetrahedral sites, Fe, Zn, Mn, Li, and Cr 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 camera. 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 — $ 83,173 — 02-2
S. Perkowitz - Physics Department
Phone: (404)-329-6584

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 — $ 56,000 — 03-1
L. Mandelkern - Dept. of Chemistry
Phone: (904)-644-2054

Studies of energy effects occurring in the crystal-liquid transition of oriented macromolecular systems. Equilibrium melting temperature-stress relations; kinetics of crystallization and melting under uniaxial and biaxial stress; a description of the morphological forms that result, and their influence on mechanical properties. Optimization of the functioning of mechanochemical systems of polymers.

351. METAL DISSOLUTION KINETICS IN ORGANIC SOLVENTS USING ROTATING RING-DISC VOLTAMMETRY — $ 90,000 (15 months) — 01-3
J. R. Ambrose - Dept. of Materials Science and Engineering
Phone: (904)-392-1456

Characterization of electrochemistry of Ni-base binary alloys in alcohol solutions and 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.

UNIVERSITY OF FLORIDA

352. SYNTHESIS AND CHARACTERIZATION OF NOVEL POLYMERS FROM NON-PETROLEUM SOURCES — $120,000 — 03-3

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

Synthesis from non-petroleum sources and structural characterization of polysaccharide-based polymers for use in tertiary oil recovery with the following objectives: 1) preparation of very high intrinsic viscosity starch graft copolymers and the characterization of their structures, 2) correlation of intrinsic viscosity of these polymers with the number of grafts per starch molecule and degree of polymerization of the grafts, 3) synthesis of high intrinsic viscosity graft copolymers with a substantial polysaccharide (starch) content, and 4) preparation of polymeric materials of high intrinsic viscosity by chain extension of polysaccharides or polysaccharide graft copolymers. Experimental and theoretical studies of the dependence of shear degradation of copolymers on their molecular structures.

THE FRANKLIN INSTITUTE

353. PHYSICS OF HIGHLY ANISOTROPIC MATERIALS — $ 22,000 — 02-3

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

A theoretical study focused on manifestations of correlations in highly anisotropic materials. The relationships between spin and charge density waves, correlations in half filled bands, solitons and Hubbard model excitations, and superconductivity in one dimensional materials will be explored.

GEORGIA INSTITUTE OF TECHNOLOGY

354. THE STRUCTURE AND REACTIVITY OF HETEROGENEOUS SURFACES AND STUDY OF THE GEOMETRY OF SURFACE COMPLEXES — $140,380 (14 months) — 02-3

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

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

355. DRIFT MOBILITIES BY TIME OF FLIGHT METHODS AND TIME DEPENDENT PHOTO-TRANSPORT IN THE NANOSECOND REGIME IN AMORPHOUS SEMICONDUCTORS — $ 90,000 — 02-2
W. Paul - Division of Applied Sciences
Phone: (617)-495-2853

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.

UNIVERSITY OF HOUSTON

356. MICROSTRUCTURAL STUDIES OF HYDROGEN AND OTHER INTERSTITIAL DEFECTS IN BCC REFRACTORY METALS — $ 73,967 — 02-2
S. Moss - Dept. of Physics
Phone: (713)-749-2840

X-ray and neutron diffraction analyses of order-disorder transitions, phase changes, and occupancy sites of H and D in BCC refractory metals--Nb, Ta, V; anomalous solubility of H in V-Nb solid solutionsl interstitial-induced strain fields and Fermi surface modifications; order-disorder transitions in the K distribution in intercalated graphite.

UNIVERSITY OF ILLINOIS/CHICAGO CIRCLE

357. OXIDATION OF TRANSITION METALS IN CHLORINE CONTAMINATED ENVIRONMENTS — $ 30,800 — 01-3
M. McNallen - Dept. of Materials Engineering
Phone: (312)-996-2436

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

JOHNS HOPKINS UNIVERSITY

358. CONDENSATION PROCESSES IN COAL COMBUSTION PRODUCTS — $ 70,000 — 03-3

J. L. Katz - Dept. of Chemical Engineering
Phone: (301)-338-8484
M. Donohue - Dept. of Chemical Engineering
Phone: (301)-338-7143

Theoretical and experimental studies of complex nucleation and condensation of particles that form slag in coal combustion and gasification, with emphasis on non-equilibrium processes. MHD systems studies of thermal and electrical properties of aerosols, and on the kinetics of nucleation and chemical reactions in fly ash and silicates.

UNIVERSITY OF KENTUCKY

359. STUDIES OF THE MICROSCOPIC PHYSICAL AND CHEMICAL PROPERTIES OF GRAPHITE INTERCALATION COMPOUNDS — $ 71,053 — 02-2

P. C. Eklund - Dept. of Physics and Astronomy
Phone: (606)-258-4849

Highly oriented pyrolytic graphite (HOPG) will be intercalated with SbX_5 or SbX_3Y_2 where X and Y are halogens. Alkali metal hydride intercalates will also be made. Materials will be studied by optical reflectance, Mossbauer spectroscopy, X-ray diffraction, Shubnikov de Haas effects, magnetoresistance, Raman and infrared spectroscopy.

360. ANISOTROPIC ELASTICITY OF COAL — $ 73,000 — 01-2

P. P. Gillis - Dept. of Metallurgical Engineering and Materials Science
Phone: (606)-258-5733, 8883
A. B. Szwilski - Dept. of Civil Engineering
Phone: (606)-258-2953, 4856

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.

UNIVERSITY OF KENTUCKY (continued)

361. STRUCTURAL CHARACTERIZATION OF DISPERSED METAL CATALYSTS — $ 94,000 (16 months) — 03-3

R. J. Reucroft - Dept. of Metallurgical Engineering and Materials Science
Phone: (606)-258-8723
R. J. De Angelis - Dept. of Metallurgical Engineering and Materials Science
Phone: (606)-258-2738

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

362. ANALYTICAL STUDY OF DRAWING AND EXTRUSION OF SUPERCONDUCTING FILAMENTARY WIRE: FRACTURE PROBLEMS AND EVALUATION OF TEMPERATURE RISE — $ 99,055 — 01-5

B. Avitzur - Dept. of Metallurgy and Materials Engineering
Phone: (215)-861-4233
Y. T. Chou - Dept. of Metallurgy and Materials Engineering
Phone: (215)-861-4235

Analytical bases for extrusion and drawing processes in the fabrication of multifilament superconducting wire; analyses/understanding of failure modes, viz., central burst phenomena and temperature increases during deformation; electrical properties of finished superconducting wires; Nb_3Sn.

363. AN EXPERIMENTAL AND ANALYTICAL INVESTIGATION OF THE CREEP-RUPTURE PROCESS — $ 55,500 — 01-2

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

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

LOUISIANA STATE UNIVERSITY

364. STUDIES OF SUB-MICRON DEVICES WITH EMPHASIS ON MOS SYSTEMS — $ 57,576 — 02-3

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

Analysis of various magneto-optical phenomena in metal-oxide-semiconductor (MOS) systems. Extension of Faraday rotation studies to include multiple reflections. Emphasis will be placed on obtaining quantum corrections to the Boltzmann equation and the resulting implications for quantum transport. Localization and strong electric and magnetic field effects in two dimensional electron gas systems will be studied.

UNIVERSITY OF MARYLAND

365. ADSORPTION ON METAL SURFACES — $155,307 — 02-2

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

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

366. MICROMECHANICAL MODELLING OF MICROSTRUCTURAL DAMAGE AT ELEVATED TEMPERATURE DURING CREEP OF SUPER-ALLOYS FOR ENERGY APPLICATIONS — $153,800 — 01-2

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

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.

367. STRUCTURE AND PROPERTIES OF GRAIN BOUNDARIES — $264,270 (11 months) — 01-1

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

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.

368. INTERFACIAL AND COLLOIDAL ASPECTS OF AQUEOUS SUSPENSIONS CONTAINING OXIDIC POWDERS — $ 95,000 (15½ months) — 01-5

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

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, colloid 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.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

369. PHYSICS AND CHEMISTRY OF PACKING FINE CERAMIC POWDERS — $105,000 — 01-5
H. K. Bowen - Dept. of Materials Science and Engineering
Phone: (617)-253-6892

Application of synthesis aspects of colloid chemistry, mono-sized particlates, and paradigms for sintering to develop a scientific understanding for controlling green density. Ordered packing of monodispersed SiO_2. Sintering of ordered TiO_2 particle compacts. Theoretical models for ordered dispersions and ordered compacts. Dispersion, packing, and sintering of SiO_2.

370. BASIC RESEARCH IN CRYSTALLINE CERAMIC SYSTEMS — $650,000 (13 months) — 01-1
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

Broad program on the science of ceramic materials; MgO used as a model material; electrical, optical, dielectric properties; defect structure, kinetics, sintering and creep studies; ionic conductivity and Mg vacancy mobility in MgO; boron diffusion in SiC; characterization of grain boundary segregation in MgO; sintering of covalent (Si) materials; influence of grain size distributions and grain arrangements on grain boundary diffusion creep; STEM studies of grain boundary composition; hot stage SEM study of microstructure development; rapid quenching of solid ceramic samples; breakaway grain growth in MgO doped Al_2O_3.

371. LOW TEMPERATURE AND NEUTRON PHYSICS STUDIES — $220,264 (13 months) — 02-1
C. G. Shull - Dept. of Physics
Phone: (617)-253-4521

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 which enter a crystal at an exact Bragg angle propagate through the crystal along the Bragg planes at a drift velocity which is much less than the group velocity. Ways are being sought to exploit this effect. Ways are also being sought to use neutron interferometry to test nonlinear variants of wave mechanics. Effect of interferometer rotation; nature of coherent wave front in interferometer; single and multiple slit Fresnel diffraction patterns.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

372. A BASIC STUDY OF HEAT FLOW IN FUSION WELDING — $ 87,000 — 01-5

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

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; corroborative experiments; material-low alloy steels.

373. HIGH TEMPERATURE PROPERTIES AND PROCESSES IN CERAMICS: THERMOMIGRATION — $ 40,000 — 01-3

B. J. Wuensch - Dept. of Materials Science and Engineering
Phone: (617)-253-6889

Effects of large temperature gradients on atomic transport behavior, defect structure, and resulting physical properties of ceramics such as KCl, UO_2, FeO, and MgO solutions. Study of principles of atomic transport due to driving forces other than composition gradients by: (a) experiments on well-defined systems with measurable boundary conditions, (b) analysis and solutions of thermomigration relations for the time dependent case, (c) examination of the assumption of local electrochemical equilibrium during the transport processes, and (d) separating the coupling coefficient into well defined kinetic and thermodynamic terms and into those which are truly reversible in nature.

374. FUNDAMENTAL INVESTIGATIONS OF THE OXIDATION OF ALLOYS IN MULTICOMPONENT GASEOUS ENVIRONMENTS — $126,200 — 01-3

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

Oxidation of Cr and Fe-Cr alloys in gases over a range of O:S potentials; differences in Cr_2O_3 formation kinetics and structure depending upon substrate crystallographic orientation; techniques used: thermogravimetry, STEM, SAM.

UNIVERSITY OF MASSACHUSETTS

375. SYNTHESIS OF METASTABLE SUPERCONDUCTING COMPOUNDS BY ION IMPLANTATION AND ELECTRON BEAM MELTING AND SPIN QUENCHING — $ 46,000 — 02-2

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

This work is concerned with the use of ion implantation to form metastable phases - in particular the formation of metastable A-15 superconductors. It addresses the possibility of epitaxial recrystallization of the implanted layer on the A-15 substrate after furnace annealing or electron beam melting. Spin quenching is considered for forming ductile amorphous superconductors.

376. EROSION OF STRUCTURAL CERAMICS — $ 28,130 (8½ months) — 01-5

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

Erosion behavior and related strength degradation of Al_2O_3, Si_3N_4, and SiC to 1200°C. Assessments 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

377. STUDIES ON AGE-HARDENING IN SPINODALLY MODULATED ALLOYS - EXPERIMENTAL AND THEORETICAL — $ 54,000 (10 months) — 01-2

K. N. Subramanian - Dept. of Metallurgy, Mechanics and Materials Science
Phone: (517)-355-2211, 5397
M. Kato - Dept. of Metallurgy, Mechanics and Materials Science
Phone: (517)-355-0294

Structure-property relationship and age-hardening mechanism 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

378. ENVIRONMENT-INDUCED EMBRITTLEMENT: EFFECTS OF IMPURITY SEGREGATION AND STATE OF STRESS — $118,000 (17 months) — 01-2

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

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

379. SURFACE-PLASMON EXPLORATION OF MULTILAYER PHYSISORBED AND CHEMISORBED FILMS ON METAL SUBSTRATES — $ 46,000 — 02-2

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

Measurements of the dielectric properties of adsorbed films by means of the loss associated with surface plasmon excitations, to study submonolayer to multilayer adsorbed gas films and hence probe a variety of phenomena in two and three dimensions. Measurements will be made on both noble gas films and nonspherical molecules such as CO on metals where orientation effects should be easily detectable.

380. EFFECT OF CRYSTALLIZATION OF GRAIN BOUNDARY PHASE ON THE HIGH TEMPERATURE STRENGTH OF SILICON NITRIDE CERAMICS — $64,597 — 01-1

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

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.

UNIVERSITY OF MICHIGAN (continued)

381. A SYSTEMATIC APPROACH TO INTER-CRACKING MECHANISMS IN AUSTENITIC ALLOYS THROUGH GRAIN BOUNDARY CONTROL — $100,000 (15 months) — 01-2
G. S. Was - Dept. of Nuclear Engineering
Phone: (313)-763-4675

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

382. NEAR NEIGHBOR SEPARATIONS OF SURFACE ATOMS — $ 55,000 — 02-2
P. I. Cohen - Dept. of Electrical Engineering
Phone: (612)-373-3025

Techniques are being developed to determine the nearest neighbor distances of atoms at the surfaces of solids by measurement of the extended fine structure in the excitation probability of core level electrons by an incident electron beam. Study will be initially made of oxygen on a Ni(111) surface in order to test the method.

383. EXPERIMENTAL STUDY OF THE THERMODYNAMICS OF THIN FILMS AND SURFACES — $ 95,000 — 02-2
A. M. Goldman - School of Physics
Phone: (612)-373-5480
E. D. Dahlberg - School of Physics
Phone: (612)-373-3358

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)

384. A MICROSTRUCTURAL APPROACH TO FATIGUE CRACK PROCESSES IN POLYCRYSTALLINE BCC MATERIALS — $ 64,000 — 01-2

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

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 effect; 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; techniques used: electron channeling, TEM, SEM.

385. HEAT CAPACITY AND OPTICAL STUDIES ON LIQUID CRYSTALS — $ 34,955 — 02-2

Cheng-cher Huang - School of Physics and Astronomy
Phone: (612)-376-2628

Heat capacity and optical property measurements will be carried out in the vicinity of the smectic A - smectic C and smectic C-tilted hexatic phase. These liquid crystal systems lack long-range inter and intra-plane positional order and are excellent systems to test defect mediated melting theories. Collobrative x-ray structure studies will provide supportive microscopic information on the same samples.

386. CORROSION RESEARCH CENTER — $900,000 — 01-1

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

Research and technology transfer in corrosion; multidisciplinary approach to corrosion research; theory of solid-fluid interfaces; plasma-sprayed coatings; adhesion of polymeric coatings; laser surface modification; plasma-processed polymer coatings; the healing process at polymer-polymer interfaces, desorption of H_2 as a chemical probe of the partial oxidation of Zn surfaces, corrosion fatigue of iron and titanium alloys; hydrogen trapping in titanium alloys; stress corrosion resistance of polymer glasses containing a rubber-reinforced ductile phase; stress corrosion cracking of electroslag refined 316 stainless steel; protection of surfaces via covalent organometallic transition metal complexes; infrared laser-induced reactions at solid-gas interfaces; reduction and cycling fatigue of oxide films; measurements of the oxidation state of iron in thin films with Auger electron and X-ray spectroscopy.

UNIVERSITY OF MISSOURI

387. DEVELOPMENT AND CHARACTERIZATION OF HIGH TEMPERATURE ELECTRICALLY CONDUCTING OXIDES — $105,000 — 01-3

H. E. Anderson - Dept. of Ceramic Engineering
Phone: (314)-341-4886, 4401
C. A. Sorrell - Dept. of Ceramic Engineering
Phone: (314)-341-4403

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 oxies 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.

388. ELECTRONIC PROPERTIES OF AMORPHOUS SILICON DIOXIDE AND METALLIC IONS IN SILICATE GLASSES — $ 40,000 (13 months) — 01-1

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

Theoretical study of the electronic properties of amorphous SiO_2, SiO_x, silicon based ceramic crystals, silicate glasses and impurity ions and defect centers in glasses. Combination of computer modelling for structures and quantum mechanical calculation of electron states by the OLCAO method. Development of theoretical methods and computer codes for self-consistent calculations within the framework of the direct-space LCAO method. Electronic structure calculations for Na, Ca, and H ions in silicate glasses using both the cluster and the quasi-periodic giant cell approach and comparison of the calculated local density of states with UPS and XPS measurements underway at Argonne National Laboratory. Electronic structure calculation on alkali silicate crystals such as Li_2SiO_3, $Li_2Si_2O_5$, $Na_2H_2SiO_2$, and β-$NaAlSiO_4$.

NATIONAL BUREAU OF STANDARDS

389. INTERAGENCY PROGRAM FOR SUPPORT OF CRITICAL DATA COMPILATIONS — $200,000

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

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 equilibrium data evaluation and compilation represent the principal thrust of this program.

NEW MEXICO INSTITUTE OF MINING AND TECHNOLOGY

390. MICROSTRUCTURAL AND MECHANICAL PROPERTY STUDY OF SOLAR ENERGY COLLECTORS — $ 90,000 — 01-1
O. T. Inal - Dept. of Metallurgical and Materials Engineering
Phone: (505)-835-5229, 5519

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, and mechanical adhesion studies.

CITY UNIVERSITY OF NEW YORK, BROOKLYN COLLEGE

391. OPTICAL AND ELECTROCHEMICAL INVESTIGATION OF RUTHENIUM AND IRIDIUM AND THEIR OXIDES IN RELATION TO THEIR ELECTROCATALYTIC ACTIVITY — $ 78,770 — 03-3
F. H. Pollak - Dept. of Physics
Phone: (212)-780-5356

Studies of factors affecting behavior of 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

392. MELTING PHENOMENA INVESTIGATED BY LASER LIGHT SCATTERING — $ 86,130 — 02-2
H. Z. Cummins - Dept. of Physics
Phone: (212)-690-6921

A comprehensive program of laser light scattering experiments to explore dynamical processes associated with melting, crystallization, nucleation and sublattice melting. The experiments are closely related to three practical problems: (1) Exploring processes which limit the rate of growth of large single crystals, (2) Studying the changes in dynamical conductivity of superionic conductors during current conduction which lead to electrolyte aging, (3) Investigating changes in the elastic properties of optical materials close to the melting temperature. Raman, Brillouin, photon correlation and forced Rayleigh scattering techniques will be used.

393. ELECTRONIC AND OPTICAL PROPERTIES OF DISORDERED SYSTEMS — $ 90,000 — 02-3
M. Lax - Dept. of Physics
(212)-690-6864

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

394. STUDY OF THE FORMATION OF SURFACE FILMS: CRITICAL CONDITIONS FOR GROWTH — $ 60,000 — 01-5
F. W. Smith - Dept. of Physics
(212)-690-6963

Critical conditions for chemical vapor deposition growth of films of SiC, Si_3N_4, and SiO_2 on single crystal Si substrates are studied under ultrahigh vacuum conditions, and the high temperature interactions of C_2H_2, C_2H_4, CH_4, CO, NH_3, N_2, NO, O_2, and H_2O with clean (111) and (100) surfaces of Si are investigated. Oxide, carbide, and silicide film formation on polycrystalline W, Mo, and Ta substrates are studied with partial pressure of reactants and substrate temperature as controlled variables. Growth of silicon homoepitaxial films formed via the reaction of SiH_4 with Si (111) and (100). Analytical techniques include Auger electron spectroscopy, X-ray diffraction, scanning electron microscopy, transmission electron microscopy.

POLYTECHNIC INSTITUTE OF NEW YORK

395. PHOTOEMISSION STUDIES OF f-ELECTRON SYSTEMS: MANY BODY EFFECTS — $ 65,000 — 02-2
R. D. Parks - Dept. of Physics
Phone: (212)-643-2070

Study of mixed valent, cerium based alloys such as $Ce_{0.9-x}La_xTh_{0.1}$ by time resolved X-ray photoemission spectroscopy. Study of well characterized mixed valent systems which exhibit valence transitions with temperature and have various 4f-(5d,6s) hybridization strengths to study many body screening effects observed frequently in deep level photoemission.

STATE UNIVERSITY OF NEW YORK/STONY BROOK

396. CONSTRUCTION AND MAINTENANCE SUNY FACILITIES AT THE NATIONAL SYNCHROTRON LIGHT SOURCE — $399,100 (13 months) — 02-2
J. Bigeleisen - Dept. of Chemistry
Phone: (516)-246-7945

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)

397. SYNCHROTRON TOPOGRAPHIC PROJECT PARTICIPATING RESEARCH TEAMS — $360,000 (10 months) — 01-1
J. C. Bilello - Dept. of Materials Science and Engineering
Phone: (516)-246-5983

Synchrotron X-ray diffraction topography to investigate plastic flow under multiaxial stresses and characterize the deformed solid state, hydrogen related fracture, hydrogen attack, hydride formation, protective oxide films, microradiography of voids, crystal growth and phase transitions in Heusler alloys, dislocations generated by the decomposition of pseudostable solid inorganic compounds, ion implantation, internal stress and strain distributions within superconductors, and nondestructive testing with an asymmetric crystal topographic camera and real time detectors.

398. SURFACE STUDIES; A PROPOSAL FOR A PARTICIPATING RESEARCH TEAM AT NSLS — $242,236 (20 months) — 02-2
F. Jona - Dept. of Materials Science and Engineering
Phone: (516)-246-7649, 6759

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, physiosorption 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.

NORTH CAROLINA STATE UNIVERSITY

399. DEVELOPMENT OF AN X-RAY BEAM LINE AT THE NSLS FOR STUDIES IN MATERIAL SCIENCE USING X-RAY ABSORPTION SPECTROSCOPY — $325,000 (14 months) — 02-2
D. E. Sayers - Dept. of Physics
Phone: (919)-737-2512

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.

UNIVERSITY OF NORTH CAROLINA

400. THE STRUCTURE OF NEUTRON DAMAGE IN IONIC REFRACTORY OXIDES — $ 37,811 — 01-4

J. H. Crawford, Jr. - Dept. of Physics and Astronomy
Phone: (919)-933-3013

Structure, thermal stability, and influence of charge state upon the behavior of lattice defects created by fast neutron bombardment and thermochemical treatment in refractory oxide single crystals. Experimental probes used to explore defect structure include optical absorption spectroscopy over the spectral range from vacuum ultraviolet to infrared, luminescent emission as excited by photons and ionizing radiation (X-rays and electron pulsed in the nsec region to permit time resolved spectroscopy), electron spin resonance, dimensional change measurements in the 10^{-6} range, electrical conductivity and electrical polarization measurements by both thermal depolarization and dielectric loss as a function of temperature. Materials under investigation include MgO, Al_2O_3 and $Y_3Al_5O_{12}$.

NORTHEASTERN UNIVERSITY

401. DYNAMICAL FRICTION IN CONDENSED MATTER — $ 89,490 — 02-3

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

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

402. STUDIES IN METAL-SEMICONDUCTOR INTERFACES IN CATALYSIS AND ENERGY CONVERSION — $ 91,000 — 03-1

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

Studies of catalyst-support interactions in methanation catalysis, with emphasis on chemical states of ad-atoms on semiconductor surfaces using X-ray photoemission. Measurement of the chemical states of Ni atoms dispersed on TiO_2(110) surfaces that have been prepared to give different surface oxygen-to-titanium ratios. Correlation between electron transfer from TiO_2 to Ni and O/Ti ratio on the TiO_2 surface; gas phase photo-decomposition of water.

NORTHWESTERN UNIVERSITY (continued)

403. EFFECT ON POINT DEFECTS ON MECHANICAL PROPERTIES OF METALS — $ 82,100 — 01-2
M. Meshii - Dept. of Materials Science
Phone: (312)-492-3213

Experimental and analytical investigation of low temperature flow behavior of Nb; influence of crystallographic orientation and interstitial atoms on deformation by primary vs anomolous slip; H_2 charging effects on dislocation motion and low temperature softening of Fe as well as on fracture by intergranular quasicleavage or microvoid coalescence.

404. AN INVESTIGATION OF MICRO-STRUCTURAL CHANGES IN FERRITIC STAINLESS STEELS CAUSED BY HIGH TEMPERATURE DEFORMATION — $ 63,680 (14 months) — 01-2
J. R. Weertman - Dept. of Materials Science and Engineering
Phone: (312)-492-5353

Investigation of 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.

405. INVESTIGATION OF DEEP LEVEL DEFECTS IN EPITAXIAL SEMICONDUCTING ZINC SULPHO-SELENIDE — $ 58,469 — 01-3
B. W. Wessels - Dept. of Materials Science and Engineering
Phone: (312)-492-3219

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.

NORTHWESTERN UNIVERSITY (continued)

406. BASIC RESEARCH ON CERAMIC MATERIALS FOR ENERGY STORAGE AND CONVERSION SYSTEMS — $ 71,500 — 01-1

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

Investigation of factors affecting electronic and mass transport behavior in solid electrolyte and electrode materials. Two-dimensional protonic conductors, including direct measurements of ion diffusivities by pulsed-field gradient NMR and dielectric relaxation. Mixed and divalent ion conduction in layered structures such as β"-alumina and β" gallates. Monte Carlo simulation of mixed and divalent ion conduction in β"-alumina. Study of the effect of a dispersed second (non-soluble) phase on ionic transport in solid electrolytes; synthesis and characterization of new materials which are potential candidates for solid electrodes or electrolytes in energy storage or conversion devices. Experimental effort involves measurements of ac conductivity, dc polarization, tracer diffusion, dielectric loss, and ion thermal current. Experimental techniques include infrared reflectivity , Raman and surface enhanced Raman spectroscopy, pulsed field gradient and stimulated echo NMR, and the chemical preparation and crystal growth of selected electrolyte materials. Systems under investigation include protonic conduction in β"-aluminas and β"gallates, and LiI-SiO_2 composites.

UNIVERSITY OF NOTRE DAME

407. MICROSTRUCTURAL EFFECTS IN ABRASIVE WEAR — $ 88,093 (15 months) — 01-5

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

Assessment of mechanisms controlling abrasive wear in multiphase alloys, 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

408. INFLUENCE OF NITROGEN ON THE SENSITIZATION, CORROSION, MECHANICAL AND MICROSTRUCTURAL PROPERTIES OF AUSTENITIC STAINLESS STEELS — $ 85,470 (15 months) — 01-1

W. A. T. Clark - Dept. of Metallurgical Engineering
Phone: (614)-422-2538
D. D. Macdonald - Dept. of Metallurgical Engineering
Phone: (614)-422-6255

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)

409. FUNDAMENTAL STUDIES OF HIGH TEMPERATURE CORROSION REACTIONS — $ 86,800 — 01-1
R. A. Rapp - Dept. of Metallurgical Engineering
Phone: (614)-422-6178

In-situ SEM study of oxidation of metals, initially Cu, Cu-Ni alloys and Cr; vapor phase nucleation of oxide and metal particles; spalling of oxide during thermal cycling; effect of H_2 on oxide morphology; influence of surface treatment on oxidation of Cr.

410. HYDROGEN ATTACK OF PRESSURE VESSEL STEELS — $ 61,391 — 01-2
P. G. Shewmon - Dept. of Metallurgical Engineering
Phone: (614)-422-2491

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

411. INVESTIGATION OF THE ELECTRICAL AND OPTICAL PROPERTIES OF ORGANO-METALLIC VAPOR PHASE EPITAXIAL $Ga_{1-x}Al_xAs$ AND $GA_{1-x}Al_xAs/GaAs$ INTERFACES IN SOLAR CELLS — $ 50,00 (9½ months) — 01-3
P. K. Bhattacharya - Dept. of Electrical and Computer Engineering

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 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, capacitance-voltage, Hall-effect, velocity-field, and photoluminescence.

PENNSYLVANIA STATE UNIVERSITY

412. STRUCTURAL PROPERTIES OF AMORPHOUS METALS BY RAMAN SCATTERING — $ 71,525 — 01-1
J. S. Lannin - Dept. of Physics
Phone: (814)-865-9231

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.

413. MECHANISMS OF WEAR IN SINGLE AND TWO PHASE MATERIALS — $ 60,900 — 01-5
N. H. Macmillan - Materials Research Laboratory
Phone: (814)-863-0180

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.

414. LASER PROCESSING OF CERAMICS — $ 97,000 (18 months) — 01-5
G. L. Messing - Dept. of Materials Science and Engineering
Phone: (814)-865-2262

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.

415. GRAIN BOUNDARY DIFFUSION AND GRAIN BOUNDARY CHEMISTRY OF CR-DOPED MAGNESIUM OXIDE — $ 49,889 — 01-3
V. S. Stubican - Dept. of Materials Science
Phone: (814)-865-9921

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

PENNSYLVANIA STATE UNIVERSITY (continued)

416. STUDY OF FIELD ADSORPTION USING IMAGING ATOM-PROBE FIELD ION MICROSCOPY — $ 46,654 — 02-2
T. T. Tsong - Dept. of Physics
Phone: (814)-865-2813

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.

417. STRUCTURE OF GLASSES CONTAINING TRANSITION METAL IONS — $ 81,500 (10 months) — 01-1
W. B. White - Materials Research Laboratory
Phone: (814)-865-1152

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 Raman and infrared 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 by optical absorption spectra, luminescence spectra, and vibrational bands. Hydration of glasses. Diffusion of hydrogen into and alkalies out of glasses using sputter-induced photon spectroscopy (SIPS).

UNIVERSITY OF PENNSYLVANIA

418. HIGH CONDUCTIVITY PROTON SOLID ELECTROLYTES — $ 89,934 — 03-1
G. C. Farrington - Dept. of Materials Science and Engineering
Phone: (215)-898-6642

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. Thermal stability of various compositions to be determined in dry and hydrated atmospheres, using TGA and DTA techniques. Characterization using neutron diffraction, NMR and complex impedance measurements.

UNIVERSITY OF PENNSYLVANIA (continued)

419. STUDIES RELATING TO THE HIGH CONDUCTIVITY OF INTERCALATED GRAPHITE — $109,534 — 02-2

J. E. Fischer - Dept. of Electrical Engineering and Science
Phone: (215)-898-6924

Synthesize various stages of intercalated graphite compounds. Obtain the chemical structures of these materials, measure the conductivity and optical properties, and interpret these measurements in terms of the structure and bonding characteristics. A wide variety of intercalants will be investigated, e.g., barium, AsF_5+F_2, XeF_n and bisulfate compounds.

420. MECHANISMS OF DAMAGE ACCUMULATION IN TIME DEPENDENT CYCLIC DEFORMATION — $ 61,000 — 01-2

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

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.

421. ATOMISTIC STUDIES OF GRAIN BOUNDARIES WITH SEGREGATED IMPURITIES — $ 67,900 — 01-1

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

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.

UNIVERSITY OF PENNSYLVANIA (continued)

422. ELECTROCHEMICAL INVESTIGATIONS OF NOVEL ELECTRODE MATERIALS — $105,000 — 03-2

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

Intercalation of Li, Na and K into TiS_2 to form $Li_xNa_yTiS_2$ and $Li_xK_yTiS_2$, 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.

UNIVERSITY OF PITTSBURGH

423. HIGH TEMPERATURE CORROSION OF CERAMICS — $ 61,000 — 01-3

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

Analysis 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.

PURDUE UNIVERSITY

424. ZERO-FLUX PLANES AND FLUX REVERSALS IN MULTICOMPONENT SYSTEMS — $ 75,576 — 01-3

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

Inderdiffusion 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.

PURDUE UNIVERSITY (continued)

425. FORMATION OF A PARTICIPATING RESEARCH TEAM AND THE INSTRUMENTATION FOR X-RAY DIFFRACTION AT THE NATIONAL SYNCHROTRON LIGHT SOURCE — $396,000 — 01-1

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

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.

426. STUDY OF ELECTRONS PHOTOEMITTED FROM FIELD EMISSION TIPS — $ 56,000 — 01-3

R. Reifenberger - Dept. of Physics
Phone: (317)-494-3032, 5555, 5386

Investigation of photo-induced field emitted electrons as a function of both their final state energy and the applied electric field using a tunable cw dye or an Argon laser. Energy resolved measurements of photo-field emitted electrons by means of a differential energy analyzer. Thermally activated surface diffusion of alkali adatoms on a field emission tip. Thermally-induced and laser-induced chemical reactions on small metallic surfaces.

427. MULTICOMPONENT DIFFUSION UNDER GENERAL CHEMICAL POTENTIAL GRADIENTS — $ 81,163 — 01-3

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

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.

PURDUE UNIVERSITY (continued)

428. MECHANISMS OF ELEVATED TEMPERATURE RUPTURE IN SINGLE PHASE CERAMICS — $ 88,000 — 01-2
A. A. Solomon - School of Nuclear Engineering
Phone: (317)-494-5753

Study of elevated temperature tensile creep and stress rupture in well-characterized single phase ceramics in terms of rate contolling mechanisms and microstructural evolution. Experimental techniques consist of (1) tensile creep using constant time 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

429. EXPERIMENTAL TESTS TO UNIFY SINTERING THEORY — $ 94,300 — 01-1
R. H. Doremus - Dept. of Materials Engineering
Phone: (518)-270-6371, 6373
R. M. German - Dept. of Materials Engineering
Phone: (518)-270-6371

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.

430. PHOTON SCATTERING AND INTERACTION ANALYSIS OF INTERFACIAL CORROSION AND CATALYSIS — $110,239 — 02-2
T. E. Furtak - Dept. of Physics
Phone: (518)-270-6545

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.

RENSSELAER POLYTECHNIC INSTITUTE (continued)

431. MOLTEN CARBONATES: MICROWAVE STUDIES OF THE VAPOR STATE — $ 80,000 — 03-3
C. W. Gillies - Dept. of Chemistry
Phone: (518)-270-6341

Microwave spectroscopic studies of the vapor above pure and mixed melts of lithium, sodium and potassium carbonates in the temperature range of 650-700°C. Evaluation of optimum operating parameters and electrolyte compositions in fuel cells.

432. PROTECTIVE OXIDE FILMS — $ 66,000 (10 months) — 01-3
R. K. MacCrone - Dept. of Materials Engineering
Phone: (518)-270-6495
S. R. Shatynski - Dept. of Materials Engineering
Phone: (518)-270-6448

Study of both point defects, impurities, and grain boundaries in films of the protective metal oxides NiO and Al_2O_3. Techniques include both discontinuous and continuous thermogravimetric analysis, electron paramagnetic resonance, photocoustic spectroscopy, internal friction, magnetization, and two point electrical conductivity for the purpose of obtaining a more precise understanding of the oxidation process.

433. LOCALIZED CORROSION AND STRESS CORROSION CRACKING BEHAVIOR OF STAINLESS STEEL WELDMENTS — $130,000 — 01-1
W. F. Savage - Materials Division
Phone: (518)-270-6448
D. J. Duquette - Materials Division
Phone: (518)-270-6448

Corrosion of 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; TEM and SEM techniques; work to be started on ferritic stainless steels also; role of surface films.

RENSSELAER POLYTECHNIC INSTITUTE (continued)

434. PROPERTIES OF GLASSES WITH HIGH WATER CONTENT — $100,000 (15 months) — 01-3

M. Tomozawa - Dept. of Materials Engineering
Phone: (518)-270-6451
E. B. Watson - Dept. of Geology

The effects of dissolved water upon physical, chemical, and transport properties of select glass compositions containing up to 14 wt. % water. These unusual high water content glasses are prepared under combined pressure-temperature conditions of 3 kbar and 800°C. Radiation effects, chemical durability, diffusion, mechanical strength, electrical conductivity, ion transport processes, phase separation, differential thermal analysis, thermogravimetric analysis, and electron spin resonance.

RICE UNIVERSITY

435. A STUDY OF THE KINETICS AND THERMODYNAMICS AND HYDROGEN IN PD-BASED ALLOYS — $ 55,000 — 01-3

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

Systematic measurements of the solubility, thermodynamic properties, and migration 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.

436. ELECTRON SPIN POLARIZATION EFFECTS IN LOW ENERGY ELECTRON DIFFRACTION, ION NEUTRALIZATION AND METASTABLE ATOM DEEXCITATION AT SOLID SURFACES — $138,521 — 02-2

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

Will use PLEED (polarized LEED) to study surfaces; e.g., Ni with Te adsorbed and W with H adsorbed. 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

437. FRACTURE TOUGHNESS PROCESSES — $ 84,826 — 01-2
S. J. Burns - Dept. of Mechanical and Aerospace Sciences
Phone: (716)-275-4082

Studies of macrocrack-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.

438. DIFFUSIONAL CREEP OF MULTI-COMPONENT SYSTEMS — $ 86,874 — 01-2
J. C. M. Li - Dept. of Mechanical and Aerospace Sciences
Phone: (716)-275-4038

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

439. SINTERING PHENOMENA OF NON-OXIDE SILICON COMPOUNDS — $108,025 — 01-1
D. R. Clarke
Phone: (805)-498-4545
F. F. Lange
Phone: (805)-498-4545

Investigation of parameters affecting powder consolidation and sintering that lead to microstructural inhomogeneities in Si_3N_4 based alloys. Non-aqueous electrolytic dispersion of Si_3N_4 powders and the establishment of zeta potential conditions for their optimum dispersion. Selection procedures for narrow powder size dispersions. Packing uniformity and porosity distribution of consolidated casts and their relationship to properties of the parent colloidal suspension. Raman microprobe spectroscopy and STEM and analytical electron microscopy. Electron energy loss spectroscopy in collaboration with N. J. Zaluzec at ANL.

RUTGERS UNIVERSITY

440. METAL ATOM DIFFUSION IN AMORPHOUS SILICA AND AT THE SILICA SURFACE — $ 51,152 (10 months) — 01-3
S. H. Garofalini - Dept. of Ceramics
Phone: (201)-932-2124

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 Pd, Pt, or Ag on amorphous silica surfaces to determine the effects of local structure.

441. HIGH PRESSURE ELECTRON RESONANCE STUDIES OF ELECTRONIC, MAGNETIC AND STRUCTURAL PHASE TRANSITIONS — $100,000 — 02-2
J. H. Pifer - Dept. of Physics
Phone: (201)-932-2522
M. C. Croft - Dept. of Physics
Phone: (201)-932-2524

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

UNIVERSITY OF SOUTHERN CALIFORNIA

442. ELECTRICAL AND MECHANICAL PROPERTIES OF OXIDE CERAMICS — $132,000 (17½ months) — 01-3
F. A. Kröger - Dept. of Materials Science
Phone: (213)-743-6224

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)

443. GRAIN BOUNDARY SLIDING AND DEFORMATION MECHANISMS DURING HIGH TEMPERATURE CREEP — $103,000 — 01-2

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

Measurement of creep and grain boundary sliding in metals--Al and Cu, and their alloys--and in alkali halides--KBr; 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; creep parameters for polycrystalline KBr and relationship to lattice vs dislocation core diffusion.

SOUTHERN ILLINOIS UNIVERSITY

444. METALLIC GLASSES AND NON-EQUILIBRIUM PHASES AS NEW CATALYSTS IN ENERGY CONVERSION SYSTEMS — $ 72,900 — 01-1

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

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

445. THE STUDY AND MODELLING OF HIGH TEMPERATURE FATIGUE CRACK PROPAGATION IN AUSTENITIC STAINLESS STEEL — $ 50,000 — 01-2

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

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)

446. CHARACTERIZATION AND ANALYSIS OF CAVITY DEVELOPMENT DURING CREEP OF CERAMICS AT ELEVATED TEMPERATURES — $ 75,000 — 01-2

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

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. 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} 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

447. SUPERCONDUCTING PROPERTIES OF ELECTRON-BEAM EVAPORATED MATERIALS — $153,931 — 02-2

M. R. Beasley - W. W. Hansen Laboratories of Physics
Phone: (415)-497-0215

This is a study of the high magnetic field properties of superconducting films prepared using electron beam coevaporation techniques. Materials studied are mainly A15 structure compounds such as Nb_xSn and V_xSn where x is near 3. Ternary substitutions such as Al for Sn and Fe for Nb are also of interest. Measurements are made of superconducting parameters, such as T_c and dH_{c2}/dT. Mechanical properties such as strain tolerance, micro-hardness and high temperature ductility are studied as a function of composition and microstructure.

448. PHOTOELECTRONIC PROPERTIES OF II-VI HETEROJUNCTIONS — $147,000 (10 months) — 01-3

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

Energy parameters and transport processes that control the electrical, photoelectronic, and photovoltaic properties of II-VI heterojunctions; preparation of II-VI heterojunctions in film-on-crystal and film-on-film form; n-ZnCdS/p-CdTe, N-ZnSSe/p-CdTe, Cu_2S/CdS, ZnO/CdTe, ITO/CdTe; measurements of J-V curves in dark and light; junction capacitance; surface photovoltage; Schottky-barrier formation; spectral response; diffusion lengths; scanning transmission electron microscopy and high resolution TEM analysis of heterojunction interfaces; lattice resolution; electron microdiffraction; Auger analysis; vacuum evaporation; spray pyrolysis; rf sputter deposition, magnetron sputtering, and chemical vapor deposition, and closed-space vapor transport techniques.

STANFORD UNIVERSITY (continued)

449. MODELLING OF DEFORMATION AND FRACTURE IN HIGH-TEMPERATURE STRUCTURAL MATERIALS — $153,000 (11 months) — 01-2

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

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, 2¼ Cr-1 Mo steel and Al alloys.

450. THE USE OF SURFACE ACOUSTIC WAVES TO STUDY SMALL FATIGUE CRACKS — $100,000 — 01-5

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

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; correlation of crack propagation rate, crack closure stress, and cyclic stress ratio.

451. MECHANISMS AND MECHANICS OF HIGH TEMPERATURE FRACTURE OF MATERIALS — $ 61,952 — 01-2

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

Study of creep deformation, cavitation, and cracking in metals--principally Cu; dependence of cavity nucleation and growth on grain boundary segregation, plastic deformation, and surface and grain boundary diffusion; mechanisms controlling breakdown of power law creep at high strain rates; grain boundary segregation effects on creep.

STEVENS INSTITUTE OF TECHNOLOGY

452. STUDIES OF MAGNETISM AND EXCHANGE SCATTERING IN SOLIDS USING SYNCHROTRON RADIATION AND SPIN POLARIZED PHOTOELECTRONS — $ 65,000 — 02-2

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

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

453. SURFACE CHARACTERIZATION OF CATALYTICALLY ACTIVE METAL ALLOY AND COMPOUND FILMS — $ 80,300 — 01-1

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

Defect structure of thin metal films (Pd/Cu, Cu/NaCl); analysis of Auger line shape of the adsorbate to evaluate film topography during growth; interfacial dislocations; overgrowth structure and growth mechanisms; techniques used TEM, AES, RHEED.

UNIVERSITY OF TENNESSEE

454. A COMBINED THERMODYNAMIC STUDY OF NICKEL BASE ALLOYS — $ 27,266 (6 months) — 01-1

C. R. Brooks - Dept. of Chemical and Metallurgical Engineering
Phone: (615)-974-5427

Free energy-composition curves for stable and metastable phase in nickel alloy systems as function of temperature; galvanic cell measurements at high temperatures (1100-1400^{o}K); heat capacity measurements from 4-1300^{o}K; computer generated phase diagrams and thermodynamic functions.

UNIVERSITY OF TENNESSEE (continued)

455. MODELING FOR ULTRASONIC NON-DESTRUCTIVE EVALUATION OF COLUMNAR STRUCTURES IN ANISOTROPIC MATERIALS — $107,000 — 01-5

B. R. Dewey - Dept. of Engineering Science and Mechanics
Phone: (615)-974-2487
B. F. Oliver - Dept. of Chemical, Metallurgical and Polymer Engineering
Phone: (615)-974-2421

Modeling of ultrasonic waves using finite element method; experimental ultrasonic measurements on Inconel and nickel specimens; materials preparation of nickel single crystals and bicrystals; measurement of ultrasonic transmission/reflection at bicrystal boundaries; ultrasonic measurements to be used to provide data for the finite element solutions to wave propagation; frequency dependent attenuation in single crystals.

UNIVERSITY OF TEXAS

456. POLAR FLUIDS: PHOTOEMISSION AND ELECTRONIC ENERGY LEVELS — $ 87,231 — 02-2

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

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. Will measure i-V curves and determine electronic energy levels, interfacial work functions. Concurrent theoretical work will include calculation of density of states.

UNIVERSITY OF UTAH

457. THE EFFECT OF PROCESSING CONDITIONS ON THE RELIABILITY OF CROSS-LINKED POLYETHYLENE CABLE INSULATION — $ 91,218 — 03-2

P. J. Phillips - Dept. of Materials Science and Engineering
Phone: (801)-581-8574

Studies of the internal structure of polyethylene insulation, including the effect of melting and recrystallization on the interfacial boundary between the insulation and the conducting layer. Morphology, dielectric loss spectra and treeing properties of an extensive series of miniature cables determined under carefully controlled extrusion, cross-linking and crystallization conditions. Apparatus for accelerated testing of "treeing" employed in studies of the aging process involving miniature extruded cables. Characterization using X-ray diffraction, light scattering, transmission electron microscopy and differential scanning calorimetry.

UNIVERSITY OF UTAH

458. THEORETICAL AND EXPERIMENTAL STUDY OF SOLID PHASE MISCIBILITY GAPS IN III/V QUATERNARY ALLOYS — $ 57,404 — 01-3

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

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. This includes the study, for nonequilibrium alloys, of spinodal decomposition and its effects on the electrical and optical properties of the alloys.

459. ELECTROLYTIC DEGRADATION OF LITHIA-STABILIZED β"-ALUMINA — $ 71,618 — 03-2

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

Studies of degradation of β-alumina near the melting point of Na, including effects of local enhancement of current density theory of critical current density. Improvement of wetting characteristics of molten Na by addition of benign additives. The effect of grain size on degradation of β-alumina at room temperature. Transformation toughening of β-alumina by addition of dispersed ZrO_2.

VIRGINIA POLYTECHNIC INSTITUTE AND STATE UNIVERSITY

460. FRACTURE MECHANISMS IN GLASS-CRYSTAL COMPOSITES — $ 99,392 (16½ months) — 01-2

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

Fracture mechanisms in glass-crystal composites with 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

461. HYDROGEN EMBRITTLEMENT TESTING $ 45,000 01-2
M. R. Louthan, Jr. - Dept. of Materials Engineering
Phone: (703)-961-6640

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

462. SPECTROSCOPY OF SURFACE ADSORBED MOLECULES $ 92,000 02-2
R. V. Coleman - Dept. of Physics
Phone: (804)-924-3781

Investigations of the properties of surfaces and interfaces containing molecular adsorbates using inelastic electron tunneling (IETS), photo-emission (ESCA), and Auger spectroscopies. IETS spectra will be obtained for a number of combinations of oxide substrate and metal overlayer electrode to establish the nature of the chemical and electronic inter-actions 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.

463. MAGNETIC IMPURITIES IN SUPERCONDUCTORS $ 72,587 02-3
J. Ruvalds - Dept. of Physics
Phone: (804)-924-3782

Study the origin of the exceptionally strong indirect exchange interactions among magnetic impurities in layered compounds like $NbSe_2$ and in rare-earth compounds such as LaGd, and (La,Th) Ce_x which are known to exhibit unusual electrical and magnetic properties. Extend the theory to the phenomenon of reentrant superconductivity and calculate the influence of external magnetic fields and varying temperature on the electrical resistance, magnetic susceptibility and thermodynamic properties of these compounds.

WASHINGTON UNIVERSITY

464. MICROSCOPIC DETERMINATIONS OF LATTICE AND ELECTRONIC STRUCTURES OF SOLIDS — $100,000 — 02-2
P. C. Gibbons - Dept. of Physics
Phone: (314)-889-6271

A high-flux imaging, electron energy loss spectrometer will be used for microscopic determinations of electronic excitations and atomic structure in a wide range of metallic and semiconducting materials.

UNIVERSITY OF WASHINGTON

465. NUCLEAR MAGNETIC RESONANCE STUDIES OF ION MOTION IN SOLID ELECTROLYTES — $ 74,000 (10 months) — 01-3
J. L. Bjorkstam - Dept. of Electrical Engineering
Phone: (206)-543-2177

Nuclear magnetic resonance (NMR) studies of spin-spin and spin-lattice relaxation, electric quadrupole interactions and direct diffusion measurements on the solid electrolytes β and β"-alumina, $LiI \cdot D_2O(H_2O)$ and borate glasses with mobile Ag^+, Li^+ and Na^+ ions. NMR is the primary tool; correlative studies include electrical conductivity, thermal analysis, Raman spectroscopy, X-ray analysis, dielectric properties, IR absorption, density, acoustic attenuation, Brillouin scattering and electron microscopy. Experiments are designed to provide a better understanding of fast ion transport in solids as a basis for improved electric storage batteries, in particular ion-ion and ion-lattice interactions, their relationship to structure and the nature of the "superionic state."

466. RUBBER ELASTICITY — $151,270 — 03-1
B. E. Eichinger - Dept. of Chemistry
Phone: (206)-543-1653

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 WISCONSIN

467. MICROSTRUCTURAL ANALYSIS OF ION-CONTAINING POLYMERS — $ 77,600 — 03-1

S. L. Cooper - Dept. of Chemical Engineering
Phone: (608)-262-3641 or -1092

Studies of microstructure of several ionomer systems by 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.

468. INTERACTION OF LOW ENERGY ELECTRONS WITH SURFACE LATTICE VIBRATIONS — $ 60,932 — 02-2

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

Theory of inelastic scattering of electrons by vibrating atoms and molecules at solid surfaces. Role of image potential in electron energy-loss spectroscopy (EELS) with low impact energies. Applications to H on W, and NH_3 and CO on Ni, Pt, Rh, and Ir. Theory of lattice dynamics of clean and adsorbate covered surfaces and of thermal diffuse scattering of electrons from clean transition metal surfaces. This program is strongly coupled with that of D. L. Mills, University of California/ Irvine.

469. INVESTIGATION OF AMORPHOUS METAL FILMS ON SEMICONDUCTOR SUBSTRATES — $ 60,000 — 01-1

J. D. Wiley - Dept. of Electrical and Computer Engineering
Phone: (608)-262-2233
J. H. Perepezki - Dept. of Metallurgy and Mineral Engineering
Phone: (608) 263-1678

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, Ni-Mo, 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.

SECTION C

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 700 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 (sub-nanosecond 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.

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, fluorescence, interferometry, gas phase spectroscopy, photoemission, 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. 725B
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 wavelength range (λ > 12 Å) 16 beam lines	0.7 GeV electron energy
X-ray electron storage ring	high brightness, continuous wavelength range (λ > .5 Å) 28 beam lines	2.5 GeV electron energy
	44	
Instruments		
Monochromators:		
plane grating	12 Å < λ < 1500 Å high resolution	
toroidal grating	10 Å < λ < 80 Å high intensity, moderate resolution	
Wadsworth	300 Å < λ < 3000 Å high intensity, moderate resolution	
Seya & Czerny Turner	1200 Å < λ < 12000 Å high intensity, moderate resolution	
two crystal	.04 Å < λ < 10 Å high resolution, fixed exit beam	
two crystal/two grating	2.5 Å < λ < 2500 Å high resolution, fixed exit beam	
Six circle spectrometer/ diffractometers	high positional and rotational accuracy	
Experimental stations	photoemission, magnetic circular dichroism, fluorescence, gas phase spectroscopy, microscopy, EXAFS, scattering, crystallography, topography	
Superconducting wiggler	λ > .1 Å high intensity	

Jerry Kraine
666-4061

HIGH FLUX BEAM REACTOR

Brookhaven National Laboratory
Upton, New York 11973

The Brookhaven High Flux Beam Reactor (HFBR) operates at a power of 40 megawatts and provides an intense source of thermal neutrons (total thermal flux = 0.7×10^{15} neutrons/cm^2-sec). The reactor is being upgraded to operate at 60 megawatts, which will result in a 50% increase of the thermal flux to 10^{15} neutrons/cm^2-sec, comparable to the highest flux beam reactors in the world. 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 1981 more than 150 persons visited Brookhaven to participate in experiments and more than 50 others collaborated from their home institutes. 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. 725B
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_0 <$200 meV Q range: $0.03 < Q < 10$ Å^{-1}
Biology	
Small Angle Neutron Scattering	Studies of large molecules. On cold source with 20x20 cm^2 Position sensitive area detector. Sample detector distance L < 2 meter Incident wavelength 4 Å $< \lambda_0 <$ 10 Å
Diffractometer	Protein crystallography 20 x 20 cm^2 area detector λ_0 = 1.57 Å
Chemistry	
2 diffractometers	Single crystal elastic scattering 4-circle goniometer 1.69 Å $< \lambda_0 <$ 0.65 Å
1 triple-axis spectrometer	Inelastic scattering Diffuse scattering Powder diffractometry
Nuclear Physics	
3 spectrometers	Neutron capture studies Energy range: $0.025\text{eV} < E_0 < 25\text{keV}$
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: 6×10^{14} neutrons/cm^2-sec; Fast (>1MeV) flux: 2×10^{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-372, Argonne National Laboratory, (312) 972-6800.

PERSONS TO CONTACT FOR INFORMATION

G. H. Lander, Projects Director	(312) 972-5518 FTS 972-5518
B. S. Brown, Operations Manager	(312) 972-4999 FTS 972-4999
T. G. Worlton, Scientific Secretary	(312) 972-6800 FTS 972-6800

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		Resolution	
		†Wave-vector	Energy	Wave-vector	Energy
Special Environment Powder Diffractometer (J. D. Jorgensen)	F5	0.5-40 Å^{-1}	*	0.35%	*
General Purpose Powder Diffractometer (J. Faber, Jr.)	F2	0.5-100Å^{-1}	*	0.25%	*
Single Crystal Diffractometer (A. J. Schultz)	H1	2-20 Å^{-1}	*	2%	*
Low-resolution Medium Energy Chopper Spectrometer (J. M. Carpenter)	F4	0.1-30 Å^{-1}	0-0.6 eV	0.02 K_o	0.05 E_o
High-Resolution Medium Energy Chopper Spectrometer (D. L. Price)	H3	0.3-9 Å^{-1}	0-0.4 eV	0.01 K_o	0.02 E_o
Small Angle Scattering Diffractometer (E. Epperson (a), C. Borso (b))	C1	0.001-0.3 Å^{-1}	*	0.004 Å^{-1}	*
Crystal Analyzer Spectrometer (T. O. Brun)	F1	3-16 Å^{-1}	0.02-0.5 eV	3%	2%

* No energy analysis
† Wave-vector, $K = 4\pi \sin\theta/\lambda$
(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	Vacant	6-70
C2	Polarized Neutron Exp.	6-40
C3	Solid He^3 Project	7.5-25
F6	Irradiations	6-20
H2	Irradiations	6-20
V1	Ultra-Cold Neutron Exp.	2.7-6.7

RADIATION EFFECTS Facility (Instrument Scientist)	Description
Radiation Effects Facility (T. H. Blewitt)	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

WNR/PSR SPALLATION NEUTRON SOURCE

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

The WNR/PSR (Weapons Neutron Research/Proton Storage Ring) facility is a pulsed spallation neutron source driven by the 800-MeV Los Alamos Meson Physics (LAMPF) linear accelerator. Materials science research by neutron scattering is currently carried out at the WNR using the advantages of time-of-flight methods. Available instruments include: a) a general purpose diffractometer for powder, liquid, and amorphous materials structural studies; 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 a constant Q spectrometer, a chopper spectrometer, and a resonance detector spectrometer. A proton storage ring (PSR) is under construction and by 1985 the WNR/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 research reactors. The WNR/PSR is being developed as a national facility with the selection of experiments based on scientific excellence and pertinence to DOE program goals.

USER MODE

User interactions are by collaborations with staff scientists or by research proposal to the neutron scattering group leader, R. N. Silver.

PERSON TO CONTACT FOR INFORMATION

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

(505) 667-6069
FTS 843-6069

WNR - WNR/PSR

TECHNICAL DATA

	1982	1985
Proton Source	LAMPF	LAMPF + PSR
Proton Source Current	750μA	1000μA
Proton Source Energy	800MeV	800MeV
WNR 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}

Instruments	Purpose and Description
General Purpose Diffractometer	Liquids and amorphous metals, powder diffraction wave vector $0.3\text{-}50 Å^{-1}$ resolution 0.45% powder 2% liquids
Single Crystal Diffractometer	Laue time-of-flight spectrometer wave vector $1\text{-}15 Å^{-1}$ 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 (shop, 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 ageement 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-sample distances: 0.5, 1.0. 1.5. . . ., 5.0 m
Beam size at specimen: 0.1 by 0.1 cm (fixed)
Sample-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)(expected delivery September 1982), with a high-resolution feeder microscope (JEOL 200CX) already operating. In 1983, a 200 kV analytical microscope is expected to 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. M. Simnad, Chairman, W.L. Bell, 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.

PERSON TO CONTACT FOR INFORMATION

Ms. Madeline Moore
National Center for Electron Microscopy
Building 72
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720

(415) 486-5006
FTS 486-5006

NATIONAL CENTER FOR ELECTRON MICROSCOPY

TECHNICAL DATA

Instruments	Key Features	Characteristics
KRATOS 1.5MeV Electron Microscope	Resolution 3 Å(pt-pt) environmental cell; hot,cold stages	50 hrs/week 150-1500 kV range in 100 kV steps and continuously variable. Max beam current 70 amp/cm^2. 3mm diameter specimens
Hitachi 650 kV Electron Microscope	General purpose resolution 20 Å environmental cell straining stage	Installed in 1969. Max. voltage 650 kV conventional HVEM
JEOL 200CX Electron Microscope	Dedicated high-resolution 2.4 Å (pt-pt) U.H. resolution goniometer stage only	200 kV only LaB_6 filament 2.3mm diameter specimens
JEOL 1 MeV Atomic Resolution Microscope (ARM) (available about March 1983)	Resolution $\leq$ 1.7 Å (pt-pt) over full voltage range. Ultrahigh resolution goniometer stage, ±40° biaxial tilt with height control	400 kV - 1 MeV 2.3mm diameter specimens
200 kV dedicated Analytical Electron Microscope (planned)	X-ray and energy-loss spectrometers microdiffraction (CB) high-vacuum field emission	100 kV - 200 kV state-of-the-art resolution

ARGONNE NATIONAL LABORATORY HIGH VOLTAGE ELECTRON MICROSCOPE-TANDEM FACILITY

Materials Science Division
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 form 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
9700 South Cass Avenue
Argonne, Illinois 60439

(312) 972-5109
FTS 972-5109

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^+10μ H/cm^2 (typical) Ni^+1 Pt^+0.1
Texas Nuclear 300-kV	Terminal voltage - 300 kV Energy stability - ±300 eV Current density - H^+20μA/cm^2 (typical) Ni^+2 Pt^+2
Ion Sources	Available for both accelerators Danfysik 910, 911 Sputter Duoplasmatron
Ion Beams	Any stable isotope
Beam Lines	Ion-beam interface to HVEM Beamlines and target chambers for irradiation and in beam analysis Duel-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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Oak Ridge, Tennessee 37830

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FTS 624-5066

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Oak Ridge Associated Universities
P.O. Box 117
Oak Ridge, Tennessee 37830

(615) 576-3422
FTS 626-3422

SHARED RESEARCH EQUIPMENT PROGRAM (SHaRE)

Technical Data

Instruments and Facilities	Key Feature(s)	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 micro-characterization techniques including microchemistry, microcrystallography, surface analysis, etc. A team of professionals runs the facility and its members facilitate the research.

USER MODE

Most of the research in the facility is funded by MRL contracts of U of Illinois faculty, and is carried out by graduate students, post-doctoral and faculty researchers and by the Center's own professional staff.

For the benefit of external users the system retains as much flexibility as possible. The preferred form of external usage is collaborative research through a contact 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

TECHNICAL DATA

Instruments	Key Features
Imaging Secondary Ion Microprobe Cameca IMS 3f	Mass analysed images to 0.3μ resolution 80A depth resolution
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 1500 K
Transmission Electron Microscope Philips EM400 (120 kV)	EDS, STEM heating, cooling stages
Transmission Electron Microscope JEOL 200 (200 kV)	EDX, STEM cooling stage
Scanning Transmission Electron Microscope Vacuum Generators HB5 (100 kV)	5Å probe EDX, EELS
Scanning Electron Microscope JEOL JSM 35C (35 kV)	50Å resolution EDX
Rutherford Backscattering (in-house construction) (3 MeV)	under development
X-ray Equipment Elliott 15 kW high brilliance source Rigaku 12 kW source Several Conventional Sources	4-circle diffractometer small angle camera EXAFS Lang topography powder cameras etc.

In addition to the main items listed above the Center also has other equipment: 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 are 8-5, except by special arrangement. Fully qualified users can and do use the equipment at any time of day. Several of the instruments are maintained in almost continuous (24 hour) use.

SURFACE MODIFICATION AND CHARACTERIZATION LABORATORY

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 industry, 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.

USER MODE

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 facility. Because of the tremendous interests expressed in these techniques and the broad range of existing collaborations, plans for a users' facility have been initiated. Until this program has been established, the informal arrangement will be continued. It should be emphasized that the goal of these interactions is to demonstrate the usefulness or feasibility of these techniques for a particular materials application and not to provide routine service alterations or analyses.

PERSON TO CONTACT FOR INFORMATION

B. R. Appleton or C. W. White

(615) 574-6283
FTS 624-6283

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

SURFACE MODIFICATION AND CHARACTERIZATION LABORATORY

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 single 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 versus 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 Laboratory
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. 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 includes the atmospheric combustion 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

Walter Bauer
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Sandia National Laboratory
Livermore, California 94550

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FTS 532-2994

COMBUSTION RESEARCH FACILITY - MATERIALS PROGRAM

TECHNICAL DATA

Instruments	Key Features
Raman Spectrometer	Rejects elastic light to within 100 cm^{-1} of laser time. 100 ms. temporal resolution.
Raman Microprobe	1 micron spatial resolution.
Sputter Induced Photon Spectroscopy (SIPS)	5 keV argon beam surface analysis of insulators.
Atmospheric Combustion 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 and fabrication 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.

USER MODE

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. Materials availability information can be obtained from Frederick A. Schmidt, Operations Manager, Materials Preparation Center.

PERSON TO CONTACT FOR INFORMATION

Frederick A. Schmidt
Materials Preparation Center
121 Metals Development Building
Ames Laboratory
Ames, Iowa 50011

(515) 294-5236
FTS 865-5236

MATERIALS PREPARATION CENTER

TECHNICAL DATA

Materials

Scandium
Yttrium
Lanthanum
Cerium
Praseodymium
Neodymium
Samarium
Europium
Gadolinium
Terbium
Dysprosium
Holmium
Erbium
Thulium
Ytterbium
Lutetium

Titanium
Vanadium
Chromium
Manganese
Zirconium
Niobium
Molybdenum
Hafnium
Tantalum
Tungsten

Magnesium
Calcium
Strontium
Barium

Thorium
Uranium

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 methods. 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, will be made available in the near future.

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 Labratory
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

alumina
aluminum
argon

beryllium
boron carbide
brass

carbon liquid
carbon phenolic
copper

deuterium
diamond
dry air
D-T-He mixture

gold

helium
high explosive
hydrogen

iron

krypton

lead
lithium
lithium deuteride
lithium hydride

methane
mica
molybdenum

neon
Nevada alluvium
nickel
nitrigen

oxygen

PBX-9502
platinum
polyethylene
polystyrene
polyurethane

quartz

Ross-Aller solar mix

salt
sodium
stainless steel
steam
steel

tungsten
tungsten carbide

uranium
uranium dioxide

water
westerly granite

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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.

SECTION D

Summary of Funding Levels

The summary funding levels for various research categories were determined from the index listing in Section E and estimating the percentage from the project devoted to a particular subject. There is overlap in the figures. For instance, funding for a project in diffusion in oxides at high pressure would appear in all three categories of diffusion, oxides, and high pressure.

During the fiscal year ending September 30, 1982, the Materials Sciences total support level amounted to about $94.5 million in operating funds (budget outlays) and $8.0 million in equipment funds. The equipment funds are expended primarily at Laboratories and are not shown in this analysis. Equipment funds for the Contract Research projects are included in the total contract dollars, being part of the operating budget. The following analysis of costs is concerned only with operating funds.

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.)	45.3	22.9
(b) South..... (Fla., N.C., Tenn., Va., La., Ga., Ky.)	8.6	21.6
(c) Midwest..... (Ohio, Ill., Wisc., Mich., Mo., Minn., Ind., Iowa, Kan.)	23.7	34.2
(d) West..... (Ariz., Okla., Wash., Texas, N. Mex., Calif., Utah, Colo., Idaho)	22.4	21.3
	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-).....	64.8	43.0

	Contract Research (% by $)	Total Program (% by $)
(b) Physics, Solid State Science, Solid State Physics (Office budget Activity Numbers 02-).....	27.7	44.7
(c) Chemistry, Chemicial Eng. (Office Budget Activity Numbers 03-).....	7.5	12.3
	100.0	100.0

3. By University, DOE Laboratory, and Industry:

	Total Program (% by $)
(a) University Programs (including laboratories where graduate students are involved in research to a large extent, LBL, Ames).....	34.8
(b) DOE Laboratory Programs.....	64.7
(c) Industry.....	0.5
	100.0

4. By Laboratory and Contract Research

	Total Program (%)
Ames Laboratory	7.18
Argonne National Laboratory	19.66
Brookhaven National Laboratory	14.90
Idaho National Engineering Laboratory	0.39
Illinois, University of (Materials Research Laboratory)	2.87
Lawrence Berkeley Laboratory	6.89
Lawrence Livermore National Laboratory	1.35
Los Alamos National Laboratory	3.30
Oak Ridge National Laboratory	20.11
Pacific Northwest Laboratory	2.02
Sandia National Laboratories	3.06
Solar Energy Research Institute	0.29
Contract Research	17.98
	100.00

16991
2712
19703

5. By Selected Areas of Research:

		% of Projects (Total=391)	Total Program $ (%)
(a)	Materials		
	Polymers	6.1	2.3
	Ceramics	47.3	25.0
	Semiconductors	16.4	10.1
	Hydrides	9.7	6.2
	Ferrous Metals	23.7	13.9
(b)	Technique		
	Neutron Scattering	11.8	20.0
	Theory	21.7	10.4
(c)	Phenomena		
	Catalysis	10.2	6.9
	Corrosion	13.3	10.8
	Diffusion	22.0	9.1
	Superconductivity	9.7	6.1
	Strength	20.5	9.9
(d)	Environment		
	Radiation	22.5	21.6
	Sulphur-Containing	6.1	4.0
	High Temperature	22.2	15.0

SECTION E

Index of Investigators, Materials, Techniques, Phenomena and Environment

The index refers to project numbers in Sections A and B.

INVESTIGATORS (LABORATORIES)

INVESTIGATORS (LABORATORIES)

INVESTIGATORS (LABORATORIES)

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INVESTIGATORS (LABORATORIES)

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INVESTIGATORS (LABORATORIES)

INVESTIGATORS (CONTRACT RESEARCH)

INVESTIGATORS (CONTRACT RESEARCH)

INVESTIGATORS (CONTRACT RESEARCH)

MATERIALS

MATERIALS

Metals and Alloys

MATERIALS

TECHNIQUES

TECHNIQUES

TECHNIQUES

TECHNIQUES

PHENOMENA

PHENOMENA

PHENOMENA

PHENOMENA

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ENVIRONMENT

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