DOE/ER-0064

Materials Sciences Programs

Fiscal Year 1980

Office of Basic Energy Sciences

U.S. Department of Energy
Division of Materials Sciences
Office of Energy Research

September 1980

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Division of Materials Sciences
Office of Energy Research
Washington, D.C. 20545

September 1980

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, and Advanced Energy Projects Divisions. Materials Sciences research is supported primarily at DOE National Laboratories and Universities. The research covers a spectrum of scientific and engineering areas of interest to the Department of Energy and is conducted generally by personnel trained in the disciplines of Solid State Physics, Metallurgy, Ceramics and Chemistry. The structure of the Division is given in an accompanying chart.

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

This report contains a listing of all research underway in FY 1980 together with a convenient index to the program.

Donald K. Stevens, 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 Sections A and B, listing all the projects, Section C, a summary of funding levels, and Section D, an index (the investigator index is in two parts - laboratory and contract research).

Each project carries a number (underlined) for reference purposes. The FY 1980 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

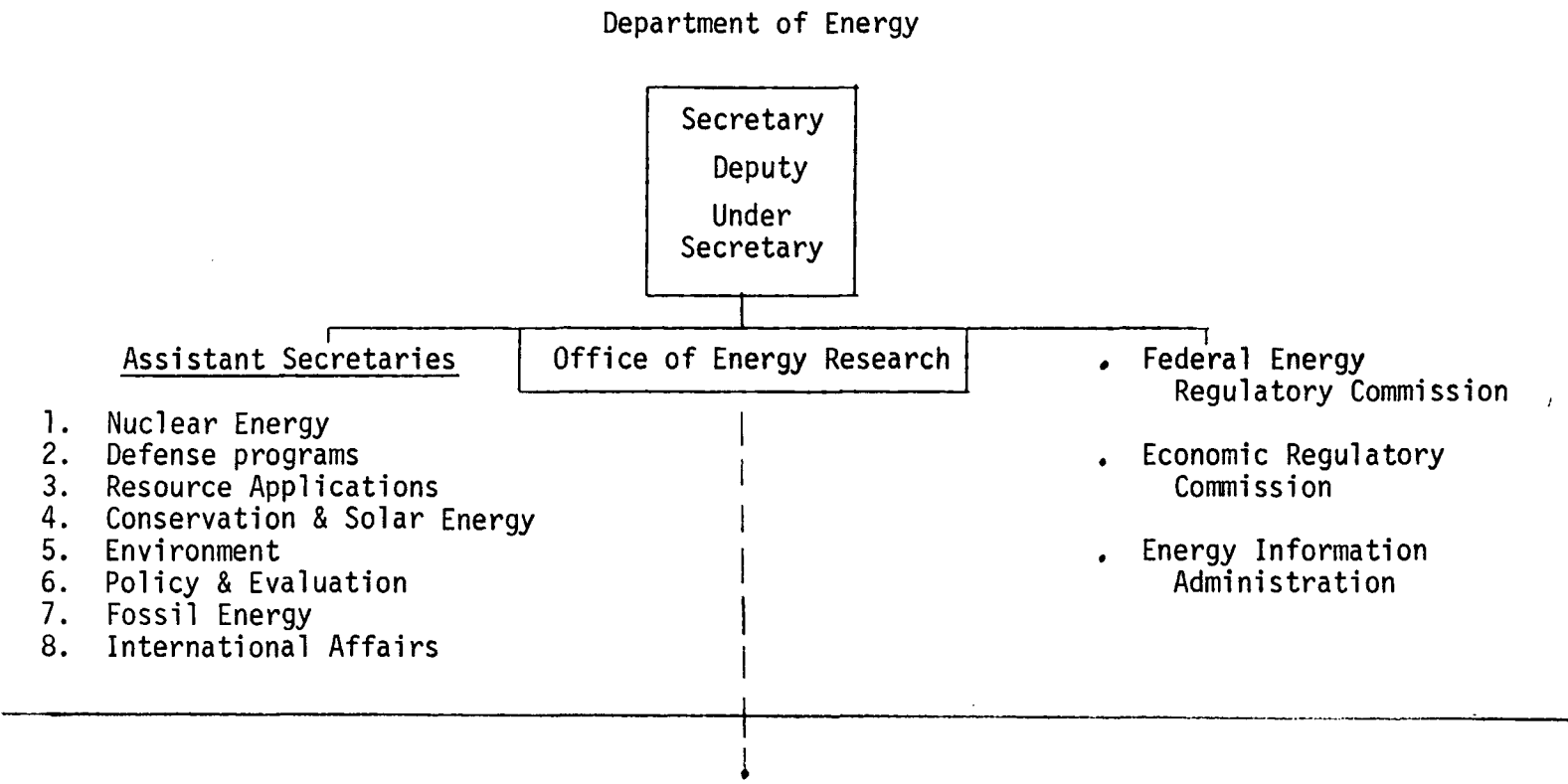
Section C summarizes the total funding level in a number of selected categories. Obviously most projects can be classified under more than one category and, therefore, it should be remembered that the categories are not mutually exclusive.

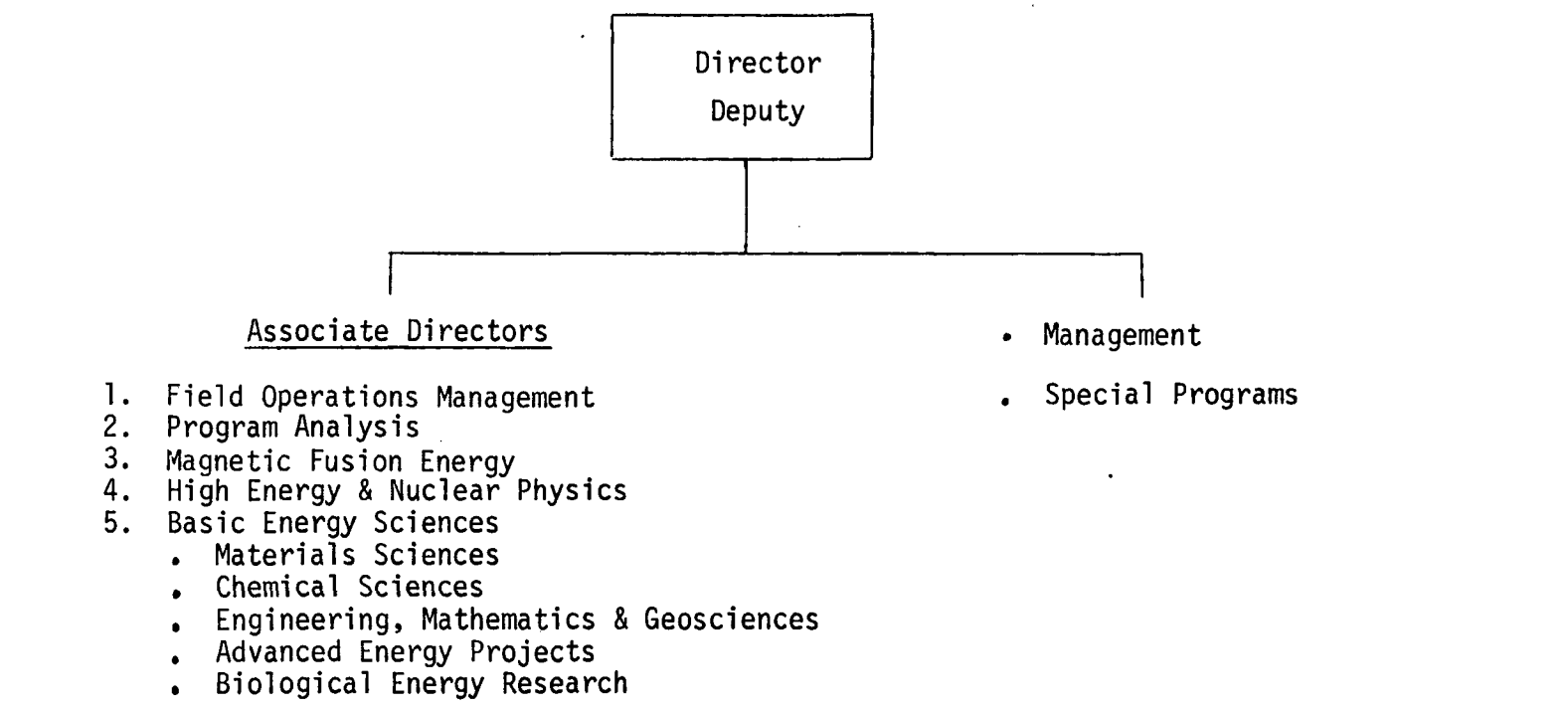
In Section D the references are to the project numbers appearing in Sections A and B and are grouped by (1) investigators, (2) materials, (3) technique, (4) phenomena, and (5) environment.

It is impossible to include in this report all the technical data available for such a large program. By the time it could be compiled it would be outdated. The best method for obtaining more detailed information about a given research project is to contact directly the investigators listed.

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

ORGANIZATION OF THE DEPARTMENT OF ENERGY



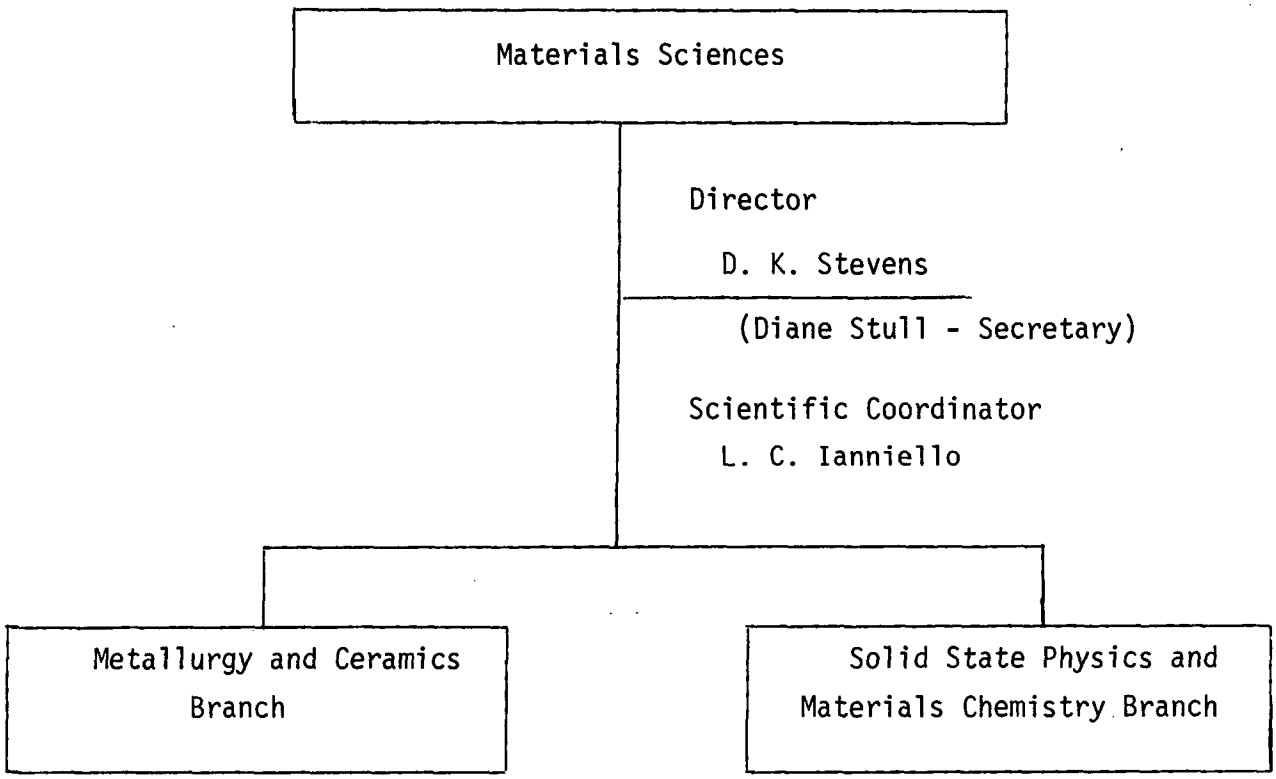


STRUCTURE

OF THE

DIVISION OF MATERIALS SCIENCES

OFFICE OF BASIC ENERGY SCIENCES



(Janet Venneri - Secretary)

Chief: L. C. Ianniello
S. M. Wolf
R. J. Gottschall
F. V. Nolfi, Jr. 1/

(Linda Twenty - Secretary)

Chief: M. C. Wittels
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Notes: 1/ On Leave from Argonne National Laboratory
2/ On Leave from Sandia Laboratories
3/ Returning to Los Alamos Scientific Laboratory 8/80
4/ Returning to Ames Laboratory 8/80
5/ On Leave from Los Alamos Scientific Laboratory

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SECTION B - Universities

SECTION C - Funding Levels

SECTION D - Index

SECTION A

Laboratories
(Primarily DOE Facilities)

This information was provided by the laboratories identified. Most projects are of a continuing nature although specific problems and some projects were concluded in FY 1980.

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

Metallurgy and Ceramics -01-
T. E. Scott - Phone: (FTS) 865-4446 or 515-294-4446

1. PHOTOVOLTAIC MATERIALS — $190,000 — 01-1
B. J. Beaudry, K. A. Gschneidner, Jr., F. A. Schmidt, R. K. Trivedi

Determination of the Schottky barrier heights of rare earth metal-silicon systems; recrystallization of amorphous silicon deposits on cubic metal substrates such as molybdenum and Fe-3 wt% Si. Precipitation of primary grains of silicon from off-eutectic liquid alloys by slowly cooling in a steep temperature gradient; high temperature electric mobility and diffusivity measurements of silicon in hafnium. Preparation of rare earth sulfides near the composition, $RS_{1.50}$ for photovoltaic conversion devices; low temperature heat capacity measurements and characterization studies of polycrystalline R_2S_3 phases.

2. RARE EARTH AND OTHER METAL PREPARATION — $180,000 — 01-1
B. J. Beaudry, O. N. Carlson, K. A. Gschneidner, Jr., F. A. Schmidt

Preparation of high purity rare earths and vanadium metals from their oxides for use in rare earth thermoelectric devices, vanadium-gallium superconductors and Al-V alloys for fusion reactor studies; metallothermic and carbothermic reduction processes are used. Ultrapurification of rare earths and, zirconium and vanadium single crystals, by electrotransport process.

3. FAST DIFFUSION — $ 20,000 — 01-1
O. N. Carlson, F. A. Schmidt

Measurement of fast diffusion of metallic solutes in thorium, lanthanum and yttrium. Use of internal friction measurements to identify type of defect associated with fast diffusion process in thorium. Correlation between activation energies for diffusion and relaxation for iron in thorium.

4. THERMOTRANSPORT AND SURFACE DIFFUSION STUDIES IN HIGH TEMPERATURE MATERIALS — $ 75,000 — 01-1
O. N. Carlson, F. A. Schmidt, R. K. Trivedi

Thermotransport studies of migration of carbon in niobium under ultra-high vacuum conditions. Measurements of high temperature surface self-diffusion of vanadium on (111) vanadium surfaces under ultra-high vacuum condition. Effect of temperature gradient on the stability of the low index surfaces of vanadium under ultra-high vacuum conditions.

AMES LABORATORY
Metallurgy and Ceramics -01- (Continued)

5. MICROSTRUCTURE STUDIES — $ 60,000 — 01-1
R. K. Trivedi

Theoretical studies of the effect of temperature and composition on the stability of microstructure, and of the morphological development of second phase with planar, spherical and dendritic interfaces. Study of morphological transition from dendritic to eutectic structure. Experimental work on dendrite and eutectic growth in Pb-Sn and Pb-Au alloys by using a controlled solidification technique. Study of morphological development in prototype transparent materials such as succinonitrile, hexachlorethane and carbon tetrachloride.

6. TEMPER BRITTLENESS IN ALLOY STEELS — $ 15,000 — 01-1
O. N. Carlson

Investigation of the effects of impurities such as tin, arsenic and antimony on the 800°F temper brittleness in Fe-2.25Cr-1Mo and Fe-9Cr-1Mo alloys in the as-cast and quenched and tempered conditions. Effect of molybdenum on the temper embrittlement of Fe-9Cr alloys.

7. HYDROGEN IN METALS — $290,000 — 01-2
C. V. Owen, S-a. Shei, T. E. Scott,
D. T. Peterson

Hydrogen embrittlement of V, Nb, Ta and their alloys; effects of C, N, and O interstitial dopants; characterization by mechanical properties, internal friction and electron microscopy. Effect of hydrogen on the mechanical properties of Sc, Y, and Lu. Hydrogen attack of steels. Diffusion, thermotransport, partial molar volumes and solubility of H and D in V alloys with Ti, Cr, or Nb. Photoelectron spectroscopy, optical properties and metallography of metal hydrides.

8. TEMPER EMBRITTLEMENT AND STRESS CORROSION STUDIES — $ 20,000 — 01-2
C. V. Owen, S-a. Shei, T. E. Scott

Near surface dislocation distribution and microstraining studies of alpha brasses in passivating and non-passivating ammoniacal solutions. Deembrittlement kinetics of temper embrittled steel doped with Sb; Auger-SIMS fracture surface analysis and depth profiling.

9. ENVIRONMENTAL EMBRITTLEMENT OF STEEL — $100,000 — 01-2
K. Sieradzki

Chlorine and H_2S gas embrittlement of steels; gas pressure effects on crack growth velocity. XPS examination of adsorption and species formed on fracture surfaces.

AMES LABORATORY
Metallurgy and Ceramics - 01- (Continued)

10. SHAPE MEMORY ALLOYS — $ 60,000 — 01-2
M. S. Wechsler

Resistivity and strain measurements during temperature cycling above and below the transformation temperature of NiTi under constant applied stress are used to determine the latent heat of transformation and the hysteresis width of the transformation for application to low-heat energy conversion devices.

11. MECHANICAL PROPERTIES OF CERAMICS — $140,000 — 01-2
W. Calderwood, M. Rasmussen, O. Hunter

Studies of HfO_2 with additives of Er_2O_3 and Ta_2O_5 designed to produce a single phase fluorite structure over the temperature range from ambient to 1300°C; elastic moduli measurements are used to detect microcracking during thermal cycling between ambient and 1300°C. Compression creep of polycrystalline Y_2O_3.

12. MATERIALS FOR SEVERE ENVIRONMENTS — $320,000 — 01-3
M. F. Berard, C. W. Chen, F. X. Kayser, J. D. Verhoeven

Production of superalloys by directional solidification; effects of composition, growth rate, and temperature gradient upon convection in Nb-Al-Mo alloys. Single and polycrystal elastic constants and yield strengths as functions of temperature for Ni_3Al. Hot extrusion methods for Fe-Si and Fe-Si-Al alloys near $Fe_3Si_{1-x}Al_x$. Structures, electrical resistivities, and corrosion of Ni-Mo alloys containing up to 20 at.% Mo. Corrosion of superalloys: kinetics and mechanisms of sulfidation of Incoloy 802 and its base alloy 22%Cr-35%Ni-Fe at 650°C. ESCA studies of the attack on Cr_2O_3 and Al_2O_3 by sulfidizing atmospheres. Cation self-diffusion, electrical conductivity, and defect structures in Er_2O_3-stabilized HfO_2.

13. AMORPHOUS MAGNETIC MATERIALS — $ 30,000 — 01-3
C. W. Chen

Fabrication of amorphous ribbons of $Fe_{82}B_{18-x}Be_x$ and $Fe_{82}B_{18-x}Au_x$ by splat cooling and magnetic properties and crystallization behavior of these ribbons. Effect of glass-forming elements on average moment of Fe atoms in these alloys.

14. SUPERCONDUCTING MATERIALS — $300,000 — 01-3
K. A. Gschneidner, Jr., O. D. McMasters, D. M. Bailey, J. D. Verhoeven, J. F. Smith

Low temperature (1-20 K) heat capacity as a function of magnetic field (0-10 T) of rare earth-based superconductors: La_3S_4-La_2S_3 and $(La_{1-x}R_x)$

AMES LABORATORY
Metallurgy and Ceramics -01- (Continued)

$(In_{1-y}M_y)_3$ with R = Sc, Y, Lu and M = Sn, Cd. Preparation and determination of superconducting transition temperatures of $(La_{1-x}Y_x)Mn_2$, La_3S_4-La_3Se_4 alloys, and $(La_{3-x}M_x)S_4$ alloys with M = Mg, Ce, Y, Th. Fabrication of Nb_3Sn-Cu superconducting composite wire by the in-situ process: casting and drawing of Nb-Cu alloys followed by Sn diffusion. Effect on microstructure of arc melted Nb-Cu alloys of graphite mold liner, liner coating materials, arc current, and arc gap voltage. Preparation of composite Cu-Fe alloys by chill casting to determine suitability for use as wire for power transmission. Thermodynamic data for Nb-Cu alloys from vapor pressures and effects of interstitial impurities on phase equilibria.

15. SINGLE CRYSTAL PREPARATION — $ 75,000 — 01-3
O. D. McMasters

Preparation of single crystals by (1) horizontal levitation zone melting, (2) vertical zone melting, (3) Bridgman, (4) strain-anneal, and Czochralski techniques including: $LaSn_3$, $CeSn_3$, Ti, Zr, Hf, Pr, α-La, γ-Ce, and 0.2 at.% Er in Au.

16. ALLOY THEORY — $ 60,000 — 01-3
B. Beaudry, K. A. Gschneidner, Jr.

Parameter development for the prediction of limits of solid solubility (>5 at.% solute--extensive; <5 at.% solute--limited) based on combination of electronegativities, atomic sizes, and electronic structures of solvent and solute.

17. HEAT CAPACITY OF RARE EARTH MATERIALS — $ 65,000 — 01-3
K. A. Gschneidner, Jr.

Intrinsic electronic specific heat coefficients and Debye temperatures from low-temperature (1-20 K) heat capacity measurements on ultrapure rare earth metals: Lu, Sc, Gd, Tb, and Y--past divergent values in the literature are attributable to high sensitivities to impurities, e.g., H and Fe. Heat capacity studies of nearly or weakly ferromagnetic materials (1-20 K; 0-10 T) to determine spin enhancement contribution: $LuCo_2$, YCo_2, Sc_3In, and Sc.

18. PHASE EQUILIBRIA COMPUTATIONS AND THERMODYNAMIC AND ELASTICITY MEASUREMENTS — $100,000 — 01-3
D. M. Bailey, J. F. Smith

DTA, EMF, and vapor pressure measurements on Li-Si and Li-Ge systems. Computer analysis of phase stability in these systems plus Li-Sn and Li-Pb. Hydrogen vapor pressures over Lu-H and Nb-Ta-H alloys and derivation of thermodynamic values for Nb-Ta system. Single crystal elastic constants of γ-Ce, of Lu, and of Lu with dilute additions of H. Anisotropic magnetic susceptibilities of single-crystal Lu with and without dilute amounts of H.

AMES LABORATORY
Metallurgy and Ceramics -01- (Continued)

19. CERAMIC PROCESSING — $ 65,000 — 01-5
G. Jordon, M. Rasmussen, M. Berard, O. Hunter

Exploratory studies of ceramic oxides produced by organic solvent dewatering of precursor gels; hydroxide gels; acetone-toluene-acetone dewatering; surface area and sintered density measurements.

20. NON-DESTRUCTIVE EVALUATION — $185,000 — 01-5
C. P. Burger, L. W. Schmerr, D. O. Thompson, L. W. Zachary

Development of a computer code using the boundary integral equation technique which will handle crack-like, 2-dimensional surface or isolated flaws. Dynamic photoelasticity used to examine the behavior of elastic Rayleigh waves as they scatter from surface or near surface flaws. Application of the displacement discontinuity stress analysis method to compute stress concentrations and stress intensities of flaws. Characterization of flaws and density gradients in ceramics. Design and construction of an ultrasonic capability for microcrack detection and characterization.

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

21. NEUTRON SCATTERING — $320,000 — 02-1
W. A. Kamitakahara, D. Khatamian, C. Stassis, J.-L. Staudenmann, J. Zarestky

Study of the thermodynamic properties and structural transformations of solids at high temperatures (Zr, Ti, Hf, Tc); electron-phonon interaction and its relation to superconductivity ($LaSn_3$, La, HfV_2, ZrV_2); electronic structure of mixed valence compounds ($CeSn_3$, $CeIn_xSn_{3-x}$, Ce_xTh_{1-x}); study of the effect of hydrogen and carbon impurities on the properties of metals (Th-H, Y-H, La-H); alkali-graphite intercalation compounds.

22. SEMICONDUCTOR PHYSICS — $160,000 — 02-2
A. J. Bevolo, H. R. Shanks

Growth and characterization of r.f. sputtered hydrogenated amorphous silicon and single crystal tungsten bronzes (Na_xWO_3, Rb_xWO_3). Hydrogenated amorphous silicon Schottky barrier solar cells; silicide formation. Auger, SIMS, and ELS studies of surfaces and interfaces of: platinized tungsten bronzes, metal-hydrides (LaH_2, TaH_x), semiconductor-metal interfaces (amorphous silicon), insulator-metal interfaces (Ta_2O_5/Ta). Sputter yield measurements, depth resolution studies, Auger studies of C, O, and N in Zr, Hf, W, and Ta, corrosion studies.

AMES LABORATORY
Solid State Physics -02- (Continued)

23. SUPERCONDUCTIVITY $360,000 02-2
D. K. Finnemore, T. Y. Hsiang
Z. Khim, J. R. Ostenson,
E. L. Wolf, R. J. Noer

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; development of superconducting composites suitable for large scale magents in the 8 to 14 Tesla range; practical studies to improve wire fabrication techniques and performance characteristics such as critical currents and ac losses.

24. OPTICAL AND SPECTROSCOPIC PROPERTIES OF SOLIDS AND LIQUIDS $400,000 02-2
T. E. Furtak, F. S. Khumalo,
D. W. Lynch, B. H. Loo, C. G. Olson,
B. Parkinson, K. K. Sharma,
F. H. Spedding

Optical properties (transmission, reflection, EXAFS, thermoreflection, thermotransmission, electroreflection) of solids in the near infrared, visible vacuum ultraviolet and soft X-ray region (using synchrotron radiation) on: transition metal alloys and compounds (e.g., FeTi), transition metal-hydrogen systems, A15 superconductors (Nb_3Ge); GaAs, layered transition metal chalcogenides ($MoSe_2$), amorphous metals. Photoemission into liquid electrolytes, electrochemical modulation spectroscopy, surface Raman scattering, and photoelectrochemistry on binary alloys susceptible to localized corrosion. 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.

25. NEW MATERIALS AND PHASES $420,000 02-2
R. N. Shelton, C. A. Swenson,
M. S. Anderson, R. G. Barnes,
S. Legvold, D. R. Torgeson

Synthesis of new ternary compounds (e.g., $LuRuB_2$) and the study of their physical properties; studies of the Chevrel phases and ternary borides; coexistence of superconductivity and long range magnetic order. High pressure heat capacity studies on solid hydrogen and deuterium; low temperature expansivity of materials (Lu and Nb) containing hydrogen. Experimental magnetic and transport properties of

AMES LABORATORY
Solid State Physics -02- (Continued

rare earth alloys. Applications of NMR to: hydrogen embrittlement of rafractory metals, (V, Nb, Ta) and alloys (V-Ti, Nb-V); trapping of hydrogen by interstitial impurities in these metals; characterization of hydrogenated amorphous silicon films.

26. MATERIALS FOR HYDROGEN STORAGE $150,000 02-2
R. G. Barnes, J. D. Corbett,
K. A. Gschneidner, Jr., B. N. Harmon,
W. A. Kamitakahara, D. T. Peterson

Interdisciplinary chemistry-metallurgy-physics program to improve understanding of metal-hydrogen interactions for development of better hydrogen-storing materials. Materials studied include rare-earth-transition metal compounds and alloys $(Y(Al, Ni)_5$-H, Y-H), low-valent and lower-dimensional compounds of Group IV and V metals (ZrClH), and alloys of Group V metals (NbV). Properties and methods include low-temperature heat capacity, X-ray and neutron diffraction, NMR, hydriding kinetics, enthalpies of hydride formation, hydrogen diffusion, UPS and XPS, and band theoretical calculations.

27. ELECTRONIC AND MAGNETIC PROPERTIES $180,000 02-3
B. N. Harmon, K.-M. Ho,
R. A. Klemm, S. H. Liu, D. Misemer

Surface electronic structure of metal electrodes (e.g. Ag), electro-reflectance, and microscopic properties of the metal-electrolyte interface. Static and dynamic properties of spin glasses. Optical and other properties of metal hydrides (ScH_x, YH_x, LaH_3). Electronic, magnetic and lattice dynamical properties of mixed valence compounds $(CeSn_3)$. Theory of phonon anomalies, lattice instabilities and soft modes in metals and their relation to the electron-phonon interaction and superconductivity (Nb, Mo, Zr, Ti). Electronic properties and chemical bonding of transition and rare earth metallic compounds $(ZrB_2$, $ZrSe_3$, ZrS, TiS, PtTe).

28. OPTICAL AND SURFACE PHYSICS THEORY $260,000 02-3
R. Fuchs, K. L. Kliewer

Optical properties of metals, semiconductors, and insulators; studies of surfaces, thin films, layered systems, small particles, and powders; effects of surface roughness, nonlocality, and local field corrections on optical properties. Raman scattering from molecules adsorbed on metal surfaces (CN on Ag). Photoemission and electroreflectance with emphasis on surface states. Photoemission into liquid electrolytes and related catalytic, electrochemical, adsorption, and corrision 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
Solid State Physics -02- (Continued)

29. SUPERCONDUCTIVITY THEORY $100,000 02-3
J. R. Clem, R. A. Klemm
V. Kogan, K. Scharnberg

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

30. X-RAY AND NEUTRON CRYSTALLOGRAPHY $185,000 03-1
R. A. Jacobson, B. J. Helland,
D. M. Bailey

Development of diffraction techniques for single crystal and non-single crystal specimens; indirect methods and refinement techniques; establishment of x-ray characterization facility; radial distribution function analysis of coal's amorphous scattering; 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.

31. METAL-METAL BONDING IN SOLID STATE MATERIALS $173,000 03-1
J. D. Corbett, R. C. Burns

Synthesis, characterization and bonding of new types of reduced inorganic compounds at high temperature (e.g., of Sc, Ti, Zr, Nb, rare earth elements); extended metal-metal bonding; catalytic activity and hydrogen storage potential of new types of reduced compounds; stress-corrosion-cracking by zirconium iodides; homopolyatomic ions (e.g., of Ge, Sn, Sb, Bi, Te); ionic intermetallic phases; crystal structures, photoelectron spectroscopy, electronic structure.

32. CHEMISTRY OF HEAVY TRANSITION METALS $152,000 03-1
R. E. McCarley, L. Brough

Chemistry of heavy transition elements, especially Nb, Ta, Mo, and W; controlled synthesis and characterization of compounds with strong metal-metal bonds in dimers, clusters, and extended structures; relation of molecular and electronic structure of such compounds to electrical

AMES LABORATORY
Materials Chemistry Division -03- (Continued)

and thermal conductivity, mechanical strength, catalytic properties, chemical reactivity, and superconductivity; condensation reactions of metal cluster compounds.

33. METALS FROM FLY ASH $145,000 03-2
G. Burnet, M. J. Murtha, N. K. Roy

Recovery of iron oxide from power plant fly ash by magnetic separation and of alumina using calcination; selective chlorination and hydrochemical processing; use of magnetic fraction for heavy media in coal preparation plants; utilization of wastes from fly ash processing plants.

34. PARTICULATE PROCESSING $255,000 03-2
L. E. Burkhart, B. C. Wong

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).

35. HIGH TEMPERATURE CHEMISTRY $210,000 03-3
H. F. Franzen, R. A. Schiffman,
J. Anderegg, I. Shilo

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

36. SURFACE CHEMISTRY AND CATALYSIS $280,000 03-3
R. S. Hansen, B. Parkinson,
K. G. Baikerikar, D. C. Johnson

Heterogeneous catalysis, reactions at clean 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; electrocatalysis at binary electrode surfaces for control of toxic or mutagenic organic molecules (nitrosoamines, polynuclear compounds) in wastes; preparation and electrochemistry of layered chalcogenide photochemical converters (e.g., MoS_2, $MoSe_2$, WSe_2).

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

Materials Science 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

37. ALLOY PROPERTIES — $649,000 — 01-1
D. J. Lam, A. T. Aldred, A. J. Arko, S. K. Chan, G. S. Knapp, B. W. Veal, P. Georgopoulos

Experimental and theoretical studies of electronic structure and its relationship to physical and chemical properties and bonding in solids; XPS and EXAFS studies of the structural and electronic properties of various metal oxides in sodium silicate glasses; crystal chemistry and electronic structure studies of ABO_4 oxides with zircon-scheelite-, monazite- and fergusonite-type crystal structure; theoretical study of EXAFS backscattering amplitude and phase-shifts for actinide elements; self-consistent, relativistic calculations of energy-level diagrams for clusters representing various crystal phases of the ABO4 compounds; dHvA, ARPES, XPS, UPS, NMR, and magnetization studies of actinide metals and intermetallic compounds to determine band structure, electronic configuration, bonding characteristic and stability of 5f electron states.

38. SCATTERING STUDIES — $311,000 — 01-1
M. H. Mueller, G. H. Lander, J. E. Epperson

Magnetic, electronic, and structural properties of actinide materials using neutron scattering; particular emphasis on measurements on single crystals using both elastic and inelastic neutron scattering; structural investigations of Pd and Nb hydrides and deuterides, and studies of storage metal hydrides of the type $LaNi_5H_6$; x-ray diffuse and neutron small-angle scattering experiments of alloy decomposition, e.g., in α-Ni-Al; small-angle x-ray scattering investigation of voids formed in oxygen doped Nb. Major involvement with design, construction, and operation at the Argonne Intense Pulsed Neutron Source; group is responsible for small-angle neutron scattering prototype at ZING-P' 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 spectrometers for inelastic studies.

39. CATALYSIS AND SURFACE STUDIES — $294,000 — 01-1
M. B. Brodsky, S. D. Bader, L. Richter

Use of intermetallic compounds as catalysts; electronic and atomic structure of intermetallic compound and transition metal surfaces; effects of gases on surface properties; surface magnetism; modification of properties in thin

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

films; low energy electron diffraction; x-ray and ultraviolet photoelectron spectroscopy; electron loss spectroscopy; Auger electron spectroscopy; thermal desorption; and surface vibrations.

40. STRENGTH AND DEFORMATION OF MATERIALS — $460,000 — 01-2
A. P. L. Turner, G. Gottstein,
U. F. Kocks, J. L. Routbort,
R. B. Schwarz

Investigation of the nature of plastic deformation of metals and ceramics; theoretical and experimental studies of the mechanisms of strengthening, deformation hardening, in situ studies of recovery and recrystallization in the HVEM; investigation of interactions between solute atoms and dislocations by internal friction and computer modeling; study of the effects of deviations from stoichiometry on deformation of oxides at high temperature; formulation of mechanistically based constitutive laws for a unified description of deformation and creep.

41. METAL PHYSICS — $1,025,000 — 01-3
R. W. Siegel, M. J. Fluss,
N. Q. Lam, J. N. Mundy,
S. J. Rothman, L. C. Smedskjaer,
D. J. Westlake, B. Chakraborty,
T. L. Marcuso

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; investigations of atomic and defect diffusivities, equilibrium defect concentrations, atomic defect interactions with one-another, with solute atoms, and with dislocations, surfaces and interfaces; hydrogen solubility limits and other properties of metal-hydrogen systems; studies of metals, including bcc refractory metals, alloys, hydrides and glasses, using positron annihilation spectroscopy, tracer diffusion, resistometry, transmission-electron and field-ion microscopy, neutron and x-ray diffraction, along with a complementary theoretical program.

42. SUPERCONDUCTIVITY: — $230,000 — 01-3
F. Y. Fradin, A. J. Arko,
G. S. Knapp, P. Georgopoulos,
T. K. Tse

Experimental research on the electron-phonon interaction in various classes of high T_c intermetallic compounds; magnetization, NMR and heat capacity studies of conduction-electron coupling in RERh4B4 compounds; EXAFS studies of anharmonic behavior and atomic disordering induced by α-particle radiation in A-15 compounds; dHvA studies of Nb_3Sb to determine the band structure at the Fermi surface; phase stability of Chevrel phase superconductors.

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

43. BASIC CERAMIC STUDIES — $532,000 — 01-3
N. L. Peterson, W. K. Chen,
J. Faber, Jr., D. Wolf,
R. J. Friauf, H. Jain,
K. Y. Liou, K. W. Schroeder

Diffusion mechanisms and point defect studies in metal oxides as a function of oxygen pressure at high temperature using tracer diffusion, conductivity, neutron and x-ray scattering techniques; ionic transport mechanisms in sodium beta-alumina; defect-solute interactions and defect clustering in oxides; theoretical studies of kinetic processes in off-stoichiometric metal oxides; x-ray scattering studies of low-energy grain boundaries in oxides; TEM studies of dislocation structures of grain boundaries in oxides; theory of grain boundary structures; diffusion mechanisms and impurity interactions in mixed alkali-silicate glasses; oxidation processes in non-stoichiometric oxides using the environmental cell in the HVEM; preparation of single crystals of metal oxides.

44. Assistance to Metallurgy and Ceramics Branch — $ 76,000 — 01-4
F. V. Nolfi

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

45. NEUTRON IRRADIATION STUDIES — $363,000 — 01-4
T. H. Blewitt, R. C. Birtcher,
M. A. Kirk, Jr., B. A. Loomis

Design and construction of the IPNS Radiation Effects Facility; development of a mechanistic understanding of the effects of neutron irradiation on the physical properties of metals; study of displacement cascades at low temperatures in ordered alloys; studies of neutron sputtering of metals; studies of ordered void arrays in tantalum and niobium in the HVEM; neutron spectrum determinations at a number of neutron sources in the U.S.; application of EXAFS to the study of defect configurations in irradiated alloys.

46. CHARGED-PARTICLE IRRADIATION STUDIES — $405,000 — 01-4
K. L. Merkle, R. S. Averback,
R. Benedek, W. E. King

Investigations of radiation effects in solids induced by energetic displacement cascades; interaction of self-interstitial atoms with impurities and defect clusters in metals by ion and electron irradiation and HVEM: damage function studies in metals by HVEM, field ion microscopy, ion irradiation and computer simulation; cascade structure in metals by TEM and computer simulation;

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

cascade energy density effects on cascade structure, on sputtering, on radiation induced segregation, and radiation enhanced diffusion at interfaces; interatomic potential calculations, low temperature diffusion of hydrogen and helium in metals.

47. KINETICS STUDIES $636,000 01-4
H. Wiedersich, P. R. Okamoto,
P. P. Pronko, L. E. Rehn,
N. J. Zaluzec, W. Wagner, Z. Wang

Investigations into mechanisms 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, laser annealing and sputtering; solute segregation to internal and external defect sinks; effects of irradiation on ordering 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 4 MV Dynamitron-2 MV Van de Graaff dual-ion-beam facility, and 300 keV ion accelerator.

48. HIGH VOLTAGE ELECTRON MICROSCOPE TANDEM FACILITY $475,000 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, specific gaseous environments and for the ion beam interface with a 300 kV ion accelerator are in use; a 2 MV tandem accelerator will be available for in-situ irradiations in FY 1981; 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 four months; installation of the 2 MV tandem accelerator and interconnection with the interface is scheduled in two phases, Phase I in FY80 with the internal positive ion source and Phase II in FY81 with the tandem mode.

49. IPNS OPERATIONS AND DEVELOPMENT $1,229,000 01-4
D. C. L. Price

The Intense Pulsed Neutron Source (IPNS) program is involved in the development of an intense pulsed spallation neutron source for materials science research with neutron scattering and irradiation techniques; during FY1980, the IPNS program operates the prototype source ZING-P'; IPNS is scheduled to begin operation in FY1981 as a national users facility.

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

50. MECHANISMS OF FAILURE OF MATERIALS — $245,000 — 01-5
A. P. L. Turner, J. L. Routbort,
R. O. Scattergood, V. K. Sethi

Investigation of particle impingement erosion of metals and ceramics; study of the erosion of corrosion product scales and the mechanisms of synergistic erosion-corrosion; theoretical and experimental studies using in-situ HVEM techniques to investigate irradiation effects on mechanical behavior; investigation of the roles of impurity segregation, cavitation and microstructural inhomogeneities on the mechanisms of elevated temperature creep and fatigue fracture.

51. NONDESTRUCTIVE EVALUATION — $225,000 — 01-5
M. H. Mueller, J. E. Epperson
E. S. Fisher, K. J. Reimann

Examination of voids, precipitates, phase separation, and strain fields from impurities in engineering materials by neutron small-angle scattering; design responsibility for small angle scattering instrument at IPNS: quantitative description of size, shape, and orientation of flaws as well as composition and stress concentrations detected by bulk-wave ultrasonics, development of ultrasonic surface wave detection of near surface defects and small defect gradients; prototype neutron resonance radiography experiment at the prototype pulsed neutron source (ZING-P').

52. CORROSION STUDIES — $245,000 — 01-5
M. B. Brodsky, K. S. Grabowski,
P. Marikar, L. E. Rehn,
L. Richter

In-situ studies of alloy corrosion in the High Voltage Electron Microscope; studies of corrosion by low and high energy electron diffraction, Auger electron spectroscopy, x-ray photoelectron spectroscopy, electron loss spectroscopy, kinetics studies and ion-beam analysis; effects of alloy modification on corrosion by ion beam implantation of minor element additions; effects of surface segregation; Ni, Ni-Cr, Ni-Al, Fe-Cr, and Fe-Al-based alloys.

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

53. NEUTRON SCATTERING RESEARCH — $1,790,000 — 02-1
T. Brun, P. Dutta, G. Felcher, J. Jorgensen, M. Misawa, C. Pelizzari, T. Postol, V. Rakhecha, F. Rotella, S. Sinha

Neutron inelastic scattering and neutron diffraction are used to study the dynamics and structure of dense fluids and amorphous solids, lattice excitations in crystals, magnetic systems, phase transitions and mechanical properties at high pressures, dynamics of hydrogen in solid and liquid metals, and molecules adsorbed on surfaces. A major effort is devoted to development of instrumentation for use with pulsed neutron sources such as IPNS. At present, work is proceeding with a prototype pulsed source. Facilities include a high-resolution powder diffractometer, a crystal analyzer spectrometer, and a chopper spectrometer. Current areas of interest include the structure and lattice dynamics of hydrides, structure and dynamics of amorphous semiconductors such as Si, magnetic scattering in magnetically ordered systems and spin glasses, two dimensional phase transitions in monolayer and sub-monolayer films, ternary superconducting systems, and valence fluctuation materials.

54. MATERIALS PREPARATION AND CHARACTERIZATION — $204,000 — 02-2
S. Susman and 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 include: anode, cathode and electrolyte compounds for high temperature batteries; ternary superconductors; orthohombic NaCN; and transition metal beryllides.

55. DEFECTS AND RADIATION DAMAGE IN OXIDES AND INSULATORS — $404,000 — 02-2
C. J. Delbecq, S. A. Marshall, W. Primak and P. H. Yuster

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; relationships of radiation damage to radiation dosages; paramagnetic resonance studies of ion probes in refractory oxides such as Y_2O_3.

56. VERY LOW TEMPERATURE STUDIES $219,000 02-2
P. Roach, L. Jedrzejek and
Y. Takano

Studies of properties of quantum liquids and solids at very low temperature. Current activities and areas of interest include: properties of superfluid phases of He^3; sound propagation, ion mobility and "texture" in new He^3 phases; adiabatic cooling by nuclear demagnetization; static and dynamic susceptibility of He^3 phases; nuclear magnetic ordering in solid He^3; and the search for triplet or p-wave superconductivity in metals.

57. SUPERCONDUCTING AND NOVEL MATERIALS $301,000 02-2
C. M. Falco, K. E. Gray, T. W. Lee,
C. S. Pang, I. K. Schuller and
J. Zasadzinski

Research in fundamental non-equilibrium processes in superconductors and in novel materials, especially technological superconductors made by sputtering. Current topics include: measurements of distribution functions in non-equilibrium superconductors; thermoelectric transport coefficients in the superconducting state; the preparation and characterization of high T_c materials by high rate sputtering; studies of gap enhancement; layered ultrathin coherent structures; transport properties measurement; two-dimensional ordering. The following applications have resulted from these studies: fault current limiter; high temperature SQUID development; superconducting transistor; superconducting filters; geophysical prospecting using SQUIDs.

58. CATALYSIS AND SURFACE STUDIES $287,000 02-2
B. Abraham, L. Iton, K. Miyano
T. Tokuhiro

Structural, electronic, dynamics, and chemical studies of zeolite catalysts for petroleum cracking and gasoline synthesis, Ziegler-Natta polymerization catalysts, and supported metal catalysts, studies of adsorbates on catalysts and model surfaces. Experimental techniques include nuclear magnetic resonance [NMR] (wide line, high power pulsed, and high resolution), electron paramagnetic resonance [EPR], extended X-ray absorption fine structure [EXAFS] (laboratory and synchrotron sources), ultrahigh vacuum [UHV]-based thermal desorption mass spectroscopy [TDMS], superconducting quantum interference device [SQUID] susceptometry, and conventional static and dynamic adsorption measurements. Programs designed to study phase transitions and order in two dimensions, as well as the dynamics of surfaces with the objective of relating these phenomena to the function of technologically and biologically important systems. The techniques employed are: the film balance, surface acoustics and light scattering. Parameters measured directly are: surface pressure (surface tension), area, capillary wave dampening and scattering of polarized light. In addition to monolayers, films and model membranes on conventional liquid substrates, films on liquid metals are also under consideration. Dynamic measurements of viscosity and tension of a liquid metal surface in equilibrium with the bulk metal, are used to provide information about surface active solutes.

59. INTERMETALLIC COMPOUNDS AND HYDRIDES $478,000 02-2
J. Cashion, G. Crabtree, B.Dunlap,
W. Johanson, H. Kierstead,
D. Niarchos, G. Shenoy, J. Viccaro

Mössbauer effect studies of ternary superconductors such as $ErRh_4B_4$ and related materials; thermodynamic, structural, electronic and magnetic properties of rare-earth (RE) hydrides, and storage hydrides such as RFe_2H_x, RFe_3H_x, RCo_3H_x. EXAFS studies of monomers and dimers of Fe isolated in argon and nitrogen matrices; studies of the Fermi surface in metals, alloys and intermetallic compounds via the de Haas van Alphen effect; resistivity and susceptibility at zero and high pressure; measurements of conduction electron effective masses; anisotropy of many-body enhancements; scattering of electrons by impurities, lattice defects and local moments. Materials of interest include Nb, Pt, Pd, actinide Materials (U_3As_4, UGe_3, RIr_3); mixed valence and other rare-earth materials (Lu, $LaSn_3$, $CeSn_3$); superconducting A-15 compounds (Nb_3Sb).

60. BASIC STUDIES OF SOLAR MATERIALS $297,000 02-2
M. Grimsditch, L. Guttman,
R. Kampwirth, J. McMillan,
J. E. Potts, D. Y. Smith

A multi-disciplinary study of the optical, electronic, thermal and structural properties of selected semiconductors of interest for solar applications. Current emphasis is on chemically-modified amorphous materials including silicon and the optical properties of heat mirrors and crystalline Si and GaAs. Topics of interest include: crystallization and annealing processes in amorphous thin films; thermal stability, photohysteresis, structure and electronic properties of chemically modified amorphous systems; studies of the random network model of amorphous materials; and theoretical limits of attainable optical properties.

61. FAST ION TRANSPORT IN SOLIDS $300,000 02-2
T. Brun, C. Delbecq, S. Marshall,
A. Rahman, J. Robinson, S. Susman,
T. Tokuhiro

Studies of basic mechanisms for ionic transport of solid electrode and electrolyte materials. The techniques include: neutron diffraction, nuclear magnetic resonance, molecular dynamics calculations and phonon structure calculations. The experimental programs are strongly coupled with material preparation procedures. Primary materials of current interest are Li-Al alloys and compounds of the NASICON family.

62. SOLID STATE THEORY AND COMPUTER SIMULATION — $530,000 — 02-3
R. Kalia, S. de Leeuw, D. Koelling, M. Parrinello, A. Rahman, J. Robinson, A. Sjolander, P. Vashishta

Molecular dynamics and the computer simulation of solids and liquids; electronic structure and properties of metals and intermetallic compounds; electron-hole plasmas in semiconductors; structure and interaction of atoms in condensed matter; the electron-phonon interaction; superconductivity in transition metals and alloys; theory of magnetism and metal-nonmetal transitions; surface phenomena including: surface structure, physisorption, chemisorption and catalysis; theoretical studies of superionic conductors including CaF_2, α-AgI and α-CuI; many-body effects of multi-component plasmas in III-V semiconducting materials; space charge layers in metal-insulator-semiconductor devices.

63. GEOTHERMAL PROSPECTING WITH SQUIDS — $230,000 — 02-5
C. Falco, M. Gershenson, I. Schuller

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

64. REGENERATIVE MATERIALS — 02-5
C. Falco

Develop heat exchanger materials for more efficient and lower temperature operation of low-temperature closed-cycle refrigerators. To be started in FY 1981.

ARGONNE NATIONAL LABORATORY

Intense Pulsed Neutron Source Program - 02

D. L. Price, Phone (FTS) 972-5518 or 312-972-5518

65. PULSED NEUTRON SOURCE DEVELOPMENT $1,100,000 02-1

D. L. Price, B. S. Brown, J. M. Carpenter,
R. L. Kustom, N. J. Swanson

This IPNS Program has the present goal of providing an intermediate-flux pulsed spallation neutron source for condensed matter research with neutron scattering and irradiation techniques. The components of the Program are: (a) the IPNS-I construction project, funded at the level of $6.4 M beginning in FY 1979, to provide an operating facility with a partial set of instrumentation by April 1981; (b) the IPNS-I Expansion construction project funded at the level of $2.4 M beginning in FY 1980, to provide additional research instrumentation; (c) an R & D program to upgrade the IPNS-I Accelerator System and to develop neutron targetry and research instrumentation required for IPNS-I; (d) a source operations program to run the ZING-P' prototype and develop operating procedures for IPNS-I, proceeding into IPNS-I operation on the completion of the construction project. Relevant research programs appear under the neutron activities of the Materials Science, Solid State Science and Chemistry Divisions of Argonne National Laboratory.

ARGONNE NATIONAL LABORATORY
Chemistry Division -03-
P. R. Fields - Phone: (FTS) 972-3570 or 312-972-3570

66. CHEMICAL STRUCTURE: NEUTRON SCATTERING, X-RAY AND EXAFS STRUCTURAL STUDIES — $820,000 — 03-01
J. M. Williams, A. J. Schultz, R. G. Teller, E. G. Sherry, M. Beno, P. Vella, T. Morrison, M. Atoji

The research emphasis is on structural and physical property studies of new materials which are of interest because of their unusual electrical or magnetic properties or because they are models of catalyst systems or show catalytic activity. The current program includes: catalytic related studies of organometallic hydride and hydrocarbon complexes and of transition metal-exchanged zeolites; one-dimensional inorganic conductors; magnetic-moment studies of rare-earth metals, alloys and compounds, and of tungsten bronzes. A major effort in support of the Intense Pulsed Neutron Source program is the design and construction of a time-of-flight, pulsed-beam, neutron diffractometer for single-crystal studies.

67. HIGH-TEMPERATURE MATERIALS CHEMISTRY — $520,000 — 03-03
K. D. Carlson, R. J. Thorn, G. E. Murch, E. G. Rauh, G. L. Bullard, S. P. S. Badwal, G. H. Winslow, J. Ziomek

The program objective is to obtain a fundamental scientific description of high-temperature materials required for the utilization of energy resources. The research focuses on the electronic and vibronic structures in terms of interatomic interactions and the relation of these interactions to the thermodynamic and transport properties of solids. Quantitative aspects of the electronic and vibronic structures are determined experimentally from photoelectron and optical spectroscopic measurements. Partial molar thermodynamic properties and transport coefficients are both experimentally measured and computer simulated using Monte Carlo techniques. Oxide and carbide ceramics are currently being investigated in relation to their applications as fuels in fast breeder reactors, as insulators, and as electrodes in high-temperature fuel cells.

ARGONNE NATIONAL LABORATORY
Chemistry Division -03- (continued)

68. PHYSICAL AND SURFACE CHEMISTRY OF ENERGY SYSTEMS — $520,000 — 03-03
D. M. Gruen, A. R. Krauss, M. J. Pellin, C. O. Steinbruchel, A. F. Wagner, R. B. Wright, G. J. Lamich, T. Foosnaes

Experimental and theoretical studies of the bombardment of surfaces with energetic particles are being conducted to identify, understand and quantify charge-transfer processes at surfaces, excitation and de-excitation mechanisms of sputtered atoms, formation of ions and molecules, effects on secondary ion fractions of monolayer coverages of oxygen on metals, oxygen partial pressure dependence of ion bombardment induced secondary photon and ion emission, determination of ionization coefficients at surfaces, and development of new techniques for measuring energy distributions of sputtered neutrals via Doppler-shifted laser fluorescence spectroscopy. Properties of Group IIIA and Group IVA element substituted AB_5 hydrides are studied. Cryochemistry and photochemistry of matrix-isolated metal atoms, clusters and molecules are studied to develop a better understanding of catalysts and of catalytic mechanisms.

69. CALORIMETRY AND THERMODYNAMICS — $140,000 — 03-03
P. A. G. O'Hare, H. E. Flotow, D. Ohlendorf

Heat capacities, entropies and enthalpy increments are measured, calculated and evaluated. These measurements are also used to detect structural changes, magnetic anomalies, and other chemical and physical phenomena. The main experimental goal of this research is to determine the heat capacities of well-characterized materials from liquid helium temperatures to 350 K. Recent emphasis has been on lanthanum-nickel and actinide hydrides, rare-earth fluorides, uranium compounds, and materials of interest in geothermal energy.

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

70. THERMODYNAMICS & CORROSION CHEMISTRY $649,000 03-02
M. Blander, P. A. G. O'Hare,
M.-L. Saboungi, G. Papatheodorou,
L. Curtiss, D. Frurip, E. Veleckis,
W. Calaway, W. Hubbard, R. Yonco

Experimental and theoretical research on the thermodynamic and corrosion properties of a variety of inorganic materials; derivation and testing of statistical mechanical theories of high temperature multicomponent solutions; prediction of thermodynamic properties and phase diagrams of sulfide, oxide, silicate and metal systems; experimental tests of theory predictions; quantum mechanical calculations of the structures and stabilities of vapor molecules; enthalpies of hydrogenation and formation of AB_5-type rare earth transition-metal alloys, both pure and substituted; thermodynamics of compounds formed between fission products and glass systems; solution properties of liquid metals and alloys; high temperature Raman spectroscopic studies of vapor and vapor complexes formed between acidic gases (e.g., Al_2Cl_6, Fe_2Cl_6) and transition metal rare earth halides and oxides; electronic absorption spectra and thermodynamics of formation of complexes; systematization of thermodynamics, elucidation of molecular structure and identity of species; evaluation of vapor transport and volatility enhancement by complexes for separation processes; kinetics and mechanisms of transition metal (Fe, Ni, Cr) corrosion in liquid metals (Li, Pb, Sn) and in ionic liquids; nature of metal-nonmetal interactions in these liquids; role of dissolved gases in electrolytes and of nonmetals in liquid metals on corrosion.

ARGONNE NATIONAL LABORATORY
Chemical Engineering Division -03-

71. ELECTROCHEMISTRY OF ENERGY STORAGE CONVERSION SYSTEMS & PROCESSES — $585,000 — 03-2
C. Melendres, Z. Nagy, M.-L. Saboungi, M. Blander, G. Papatheodorou, F. A. Cafasso T. Cape, J. Settle, J. Marr

Kinetics and mechanisms of processes occurring at cell electrodes and in electrolytes; surface, structural, and theoretical studies of these processes; in situ investigations of electrocatalysis and electrode corrosion using coupled spectroscopic (visible, IR, Raman/Mossbauer) and electrochemical techniques; study of oxygen reduction at organometallic/carbon electrodes (e.g., iron phthalocyanine and porphyrins on carbon); research on anodic corrosion and passivation of metals (e.g., Fe, Pb, Co) in aqueous and molten salt electrolytes; quantum theoretical studies on electron transfer processes at the solid/solution interface; resonance Raman spectroscopic investigations of electrochemically generated species in molten salt electrolytes; study of metal (Fe, Ni, Cu) and sulfide (FeS, NiS) dissolution/deposition reactions in molten electrolytes by galvanostatic pulse and rotating-disc electrode techniqes; measurement of transition metal and heavy metal sulfide solubilities; study of sulfide-polysulfide equilibria and complexing of cations by anionic species in molten salt electrolytes; research on fundamental chemistry of electrochemical processing.

72. CHEMISTRY OF MATERIALS — $400,000 — 03-02
P. Cunningham, R. Kumar, B. Holt, D. Drapcho, S. Siegel, T. Renner

Chemistry of atmospheric particulates; elucidation of formation mechanisms of atmospheric sulfate, nitrates, organics, and silica by stable oxygen isotope ratio measurements and other techniques; development of instrumentation and methodology for sampling and real-time characterization of particulates; phase equilibria in SO_X-NO_X-H_2O systems; thermodynamics of combustion-derived condensed-phases; kinetics of gas-solid reactions and role of structural disorder in determining these kinetics.

BROOKHAVEN NATIONAL LABORATORY
Upton, Long Island, New York 11973

Corrosion Science Group -01-
J. R. Weeks - Phone: (FTS) 666-2617 or 516-345-2617
M. Suenaga - Phone: (FTS) 666-3518 or 516-345-3518

73. INTERGRANULAR STRESS CORROSION $297,000 01-2
H. S. Isaacs, Brijesh Vyas,
M. W. Kendig, C. S. Pande, K. Sieradzki

Electrochemistry of surfaces of iron and nickel base alloys at high temperatures using an ac polarization technique. In situ study of heterogeneities of corroding surfaces using scanning ac polarization technique. Measurement of corrosion currents from a propagating stress corrosion crack using a scanning reference electrode technique. Determination of chromium depletion and grain boundary segregation in stainless steels and Inconel 600 using energy dispersive x-ray analysis attached to a scanning transmission electron microscope. Effect of temperature on the stress corrosion cracking of sensitized stainless steel in oxygenated high temperature water. The effect of sulfur containing anions on stress corrosion of sensitized stainless steels. Mechanism of electrochemical dissolution in cracks.

Materials Science Division -01-
M. Suenaga - Phone: (FTS) 666-3518 or 516-345-3518

74. BASIC PROCESSES AND MICROSTRUCTURAL PROPERTIES OF AMORPHOUS SEMICONDUCTORS $210,000 01-1
R. W. Griffith, R. R. Corderman, M. D. Hirsch,
F. J. Kampas, P. E. Vanier

Fundamental materials investigations on the electrical, optical, and microstructural properties of amorphous semiconductor thin films, with particular emphasis upon limiting processes in solar energy conversion. The basic nature of localized states and the chemical bonding of amorphous semiconductors will be explored within the dual context of: i) optoelectronic processes, and ii) microstructural manifestations. Basic processes will be investigated that underlie plasma deposition such as surface reactions involving free radicals that promote film growth. Novel approaches will be studied for passivation of defects in amorphous semiconductor films that are plasma-deposited from hydrides and/or halides.

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

75. RELATIONSHIP BETWEEN PROPERTIES AND STRUCTURES — $257,000 — 01-3
D. O. Welch, M. Suenaga, C. S. Pande, K. Itoh

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 kinetics in A15 compounds; studies by electron microscopy of lattice defects in superconducting compounds; properties of composite superconductors; new methods of fabricating superconducting materials.

76. PHYSICAL METALLURGY OF METAL HYDRIDE SYSTEMS — $410,000 — 01-3
M. A. Pick, J. R. Bethin, S. M. Heald, C. S. Pande, D. O. Welch

Studies of physical and metallurgical factors which influence the hydriding behavior of 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-hydrogen systems using optical, neutron and x-ray diffraction, EXAFS, electron microscopic, and surface sensitive techniques.

77. MATERIALS FOR ELECTROCHEMICAL ENERGY CONVERSION AND STORAGE — $70,000 — 01-3
W. E. O'Grady, S. Srinivasan

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 and x-ray photoelectron spectroscopy 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.

78. RADIATION DAMAGE — $236,000 — 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 A15's and A15 composites using internal friction and dynamical Young's modulus techniques.

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

79.	EFFECT OF MICROSTRUCTURE AND ENVIRONMENT UPON FRACTURE TOUGHNESS S. K. Hwang, D. Gan	$153,000	01-5

Fundamental study on the relationship between microstructures and fracture toughness of structural materials: microstructure changes due to fatigue and creep and various environmental atmospheres: Ni, solid solution superalloy and commercial alloys: TEM and small angle neutron scattering will be employed.

BROOKHAVEN NATIONAL LABORATORY
Department of Physics -02-
N. P. Samios - Phone: (FTS) 666-3866

80.	NEUTRON SCATTERING - MAGNETIC SYSTEMS S. M. Shapiro, J. D. Axe, C. R. Fincher, Jr., W. Thomlinson G. Shirane	$649,000	02-01

Neutron scattering studies of the structure and dynamics of magnetic materials. Spin dynamics of low-dimensional, amorphous and disordered magnetic systems; correlations in spin glasses; magnetic ordering in superconductors.

81.	NEUTRON SCATTERING - PHASE TRANSITIONS G. Shirane, J. D. Axe, S. K. Satija, S. M. Shapiro, R. Youngblood	$704,000	02-01

Neutron scattering studies of structural phase transitions and their dynamics; low-dimensional charge density waves; phase transitions and dynamics of incommensurate systems; soft modes in solids; hydrogen bonded systems.

82.	NEUTRON SCATTERING - ELEMENTARY EXCITATIONS IN SOLIDS J. D. Axe, L. Passell, G. Shirane, C. R. Fincher, Jr., C. F. Majkrzak	$650,000	02-01

Neutron spectroscopy of low-lying excited states in solids; electron-phonon interactions in metals; dynamics of mixed valence systems; lattice dynamics of metal hydride systems; anharmonic phonon effects in insulators.

83.	NEUTRON SCATTERING - PARTIALLY ORDERED SYSTEMS L. Passell, C. F. Majkrzak, S. M. Shapiro, R. Youngblood, H. Grimm	$704,000	02-01

Neutron scattering studies of short-range order and excitations in partially ordered systems: radiation damage to the structures of high temperature superconductors; dynamics of solid electrolytes; dynamics of thin superfluid ^{4}He films adsorbed on graphite; polymerization.

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

84. EXPERIMENTAL RESEARCH - SPECTROSCOPY OF SOLIDS — $464,000 — 02-02
B. C. Frazer, Y. Fujii, J. B. Hastings, M. Howells, W. C. Thomlinson, G. P. Williams

X-ray and neutron studies of structural, dynamic and electronic properties of solids. Diffuse scattering in ferroelectric phase transitions. Order-disorder in hydrogen-bonded systems. EXAFS studies with synchrotron radiation on transition metal alloy systems. X-ray studies of graphite intercalant systems. Equipment development for x-ray and VUV experiments at the NSLS facility.

85. EXPERIMENTAL RESEARCH - NATIONAL SYNCHROTRON LIGHT SOURCE, R&D — $1,132,000 — 02-02
A. van Steenbergen, M. Blume, K. Batchelor, J. B. Godel, G. Bagley, L. Blumberg, J. B. Hastings, M. Howells, H. C. H. Hsieh, S. Krinsky, M. Perlman, J. Sheehan

R&D in support of the NSLS project. This facility is the first in this country designed expressly for use of synchrotron radiation and the performance objectives for the electron storage rings are quite different from those of importance in high energy physics applications. Program involves design studies, model work, experimental testing and computer analyses to optimize performance characteristics and to develop new beam line instrumentation which permit users to take full advantage of the capabilities of this new research facility.

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

86. EXPERIMENTAL RESEARCH - PROPERTIES OF REAL SOLIDS — $403,000 — 02-02
A. N. Goland, K. G. Lynn,
J. Jean, P. W. Levy, C. L. Snead, Jr. (DEE),
W. J. Kossler, College of William and Mary,
H. H. Jorch and I. K. MacKenzie, U. Guelph, Canada,
D. O. Welch (DEE), M. S. Spergel (CUNY)

Investigations of perfect and imperfect solids by specialized experimental methods; slow-positron behavior at and near well-characterized metal surfaces and interfaces, positron bulk diffusion, positron trapping in surface states and positronium formation; studies of high-momentum core annihilations as a function of temperature, positron annihilation in technologically important metals and alloy systems; applications of μ^+SR to defect problems in metals; development of μ^+SR channel at AGS, geophysical applications of mineral thermoluminescence; determination of extra terrestrial surface compositions.

87. EXPERIMENTAL RESEARCH - ADVANCED MATERIALS SYNTHESIS AND CHARACTERIZATION — $185,000 — 02-02
A. N. Goland, D. E. Cox,
A. Moodenbaugh, J. B. Hastings,
B. C. Frazer, C. T. Prewitt (SUNY-Stony Brook),
T. Egami (U. Penn.), M. A. Anderson and
A. S. Nowick (Columbia)

Synthesis, characterization and electrical properties of inorganic materials; 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 planning for beam line at NSLS, monochromator preparation facility for NSLS.

88. EXPERIMENTAL RESEARCH - ALTERATION AND ANALYSIS OF SOLIDS BY ION BEAMS — $143,000 — 02-02
A. N. Goland, C. Clayton,
H. Herman, S. Prasad, Y. F. Wang (SUNY-Stony Brook),
M. Pick (DEE), A. Hanson, K. W. Jones,
R. W. Klaffky (NSLS), J. A. Golovchenko (Bell Labs)

Channeling, ion implantation and defect profiling in metals, alloys and nonmetals; energy loss of similarly charged heavy ions, ^{18}O profiles in alumina, alteration of electrochemical properties by ion implantation, ESCA, and TEM analysis; formation of alloys and precipitates by ion implantation; hydrogen profiling by nuclear reaction techniques; surface phenomena and thin films.

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

89. THEORETICAL RESEARCH $599,000 02-03
V. J. Emery, J. Black,
J. Davenport, G. J. Dienes,
R. A. Pelcovits, G. Reiter,
R. E. Watson, M. Blume

Phase transitions, critical and cooperative phenomena in magnetic systems, liquid helium and incommensurate structures; properties of one- and two-dimensional materials by analytic and numerical methods; metal surfaces, adsorbed films and hydrogen absorption; electronic structure of metals and alloys; x-ray and neutron scattering; properties of disordered materials and crystal defect physics.

90. PARTICLE-SOLID INTERACTIONS - RADIATION EFFECTS RESEARCH $587,000 02-04
A. N. Goland, P. W. Levy,
K. G. Lynn, P. J. Schultz, U. Guelph,
Canada; I. K. Mackenzie, U. Guelph,
C. L. Snead, Jr. (DEE), R. W. Klaffky,
Y. C. Jean

Comparison of radiation effects in metals and alloys as a function of incident neutron energy spectrum by positron-annihilation lifetime and Doppler-broadening measurements, in situ studies of electron bombarded natural and synthetic NaCl by measurements of optical absorption and radioluminescence; thermoluminescence of gamma-irradiated quartz; dislocation generation in gamma-irradiated crystals; analysis of radiation-induced conductivity in aluminum oxide; calculation of radiation damage parameters for metals and nonmetals in a deuteron-stripping type intense neutron source; planning of beam line for studies of transient photon-induced defects in solids and liquids at National Synchrotron Light Source.

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

91. ENGINEERING PHYSICS - SUPERCONDUCTIVITY — $347,000 — 02-05
A. Ghosh, Z. Ovadyahu, M. Strongin

Transport properties in superconductors in different states of disorder; tunneling into N-S layers; the nature of the superconducting transition in two dimensions; studies of crystal structure and electronic properties of Nb_3Sn layers grown on Nb.

92. ENGINEERING PHYSICS - SURFACE STUDIES — $333,000 — 02-05
M. El-Batanouny, R. J. Smith, M. Strongin, S. L. Weng

Use of photoemission to determine the properties of hydrogen on transition metals; studies of structure and structural transitions in overlayers and how hydrogen uptake in the underlying metal is affected; photoemission studies of electronic structure changes during structural transitions in overlayers; studies of the mechanism of positive ion formation during electron stimulated desorption; design and construction of VUV beam line for photoemission experiments at NSLS.

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

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

93. SCALING AND CORROSION IN ENERGY CONVERSION SYSTEMS — $140,000 — 03-1
L. A. Casper, W. F. Downs

Chemical mechanisms of scaling and corrosion; mapping of the reactivity of engineering alloy surfaces to determine sites which promote nucleation of scale components or the initiation of corrosion; acid/base structure of oxide surfaces; scale nucleation and growth at a heat-transfer rotating disk; dissolution kinetics and thermodynamics of calcite (calcium carbonate) in synthetic geothermal brines with emphasis on coupling and complex behavior in unary, binary, and ternary brines.

94. WELDING RESEARCH — $250,000 — 01-5
J. F. Key, G. R. Smolik, H. B. Smartt

Heat source/molten pool interaction studies utilizing high-speed cinematography, emission spectroscopy and infrared thermography. Process parameter, material properties, solidification structure relationships. Solidification and heat flow modeling. Post weld embrittling mechanisms; cracking tendency determinations; age hardenable nickel base alloys; influence of oxygen in the embrittlement process; publication of BES Newsletter.

95. ENVIRONMENTAL EFFECTS ON MECHANICAL PROPERTIES OF METALS
G. R. Smolik, R. M. Horton — $100,000 — 01-5

Failure mechanisms of Alloy 800H exposed to simulated coal gasification environments. Oxidation and sulfidation propensities; influences of gas composition, surface condition, grain size, cold work, thermal cycling, deformation, and the presence of crevices, cracks, and weldments.

ILLINOIS, UNIVERSITY OF
Urbana, Illinois 61801

Materials Research Laboratory -01-
C. P. Flynn - Phone: 217-333-1370

96. LOCALIZED CORROSION OF PASSIVE METALS — $ 23,000 — 01-1
R. C. Alkire

Corrosion of metals owing to fluid flow. Erosion by particle impaction and cavitation. Transport models of early growth of corrosion pits.

97. THEORY OF POLYMERS — $ 5,000 — 01-1
R. J. Gaylord

Statistics of confined polymer chains. Deformation of semicrystalline polymers, filled or reinforced elastomers, block copolymers and cross-linked networks. Scaling concepts in polymer physics. Behavior of polymer chains in the presence of surfaces.

98. SEMICONDUCTOR CRYSTAL GROWTH BY ION BEAM SPUTTERING — $ 95,000 — 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 compounds and II-IV-V_2 chalcopyrite systems.

99. DYNAMICAL STRUCTURE OF MATERIALS UNDER EXTREME CONDITIONS OF TEMPERATURE AND PRESSURE — $ 115,000 — 01-1
J. Jonas

Dynamical structure of water and electrolytes at high temperature and high pressure. Structure-property relationship in polymeric materials. Transport processes in undercooled metals and intercalated compounds. Laser Raman scattering studies of vibrational relaxation in fluids. Measurement techniques for extreme conditions of temperature and pressure.

100. CHARACTERIZATION OF COMPOUNDS AND ALLOYS — $ 90,000 — 01-1
C. A. Wert and H. L. Fraser

Development of microchemical and analytical methods on a 20 Å scale using electron energy loss and energy dispersive spectroscopies. Applications to carbides, oxides, and nitride precipitates in bcc metals. Investigation of heavy metal sulfides and oxides in coal.

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (Continued)

101. HYDROGEN BEHAVIOR IN BCC METALS — $ 140,000 — 01-2
H. K. Birnbaum

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.

102. MECHANICAL PROPERTIES OF MATERIALS — $ 40,000 — 01-2
J. Holder

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

103. MICROANALYSIS OF METALLURGICAL SYSTEMS — $ 38,000 — 01-2
R. Hutchings

Development of techniques in analytical electron microscopy. Investigation of phase transformations in metallic and metal/gas systems; multilayer oxide films and spalling.

104. COUNCIL ON MATERIALS SCIENCE — $ 51,000 — 01-2
R. J. Maurer

Acquisition of information concerning current and proposed basic research on materials and their application to problems of energy utilization.

105. OXYGEN IN REFRACTORY BCC METALS — $ 45,000 — 01-3
C. J. Altstetter

Thermodynamics and diffusion of oxygen in refractory metals using solid electrolyte cells. Metal-oxygen and oxygen-oxygen interactions in alloys.

106. STRUCTURE, CRACKING AND CORROSION OF CERAMIC GRAIN BOUNDARIES — $ 81,000 — 01-3
S. D. Brown and W. T. Petuskey

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.

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (Continued)

107. DEVITRIFICATION BEHAVIOR IN METAL-CONTAINING SILICATE GLASSES — $ 45,000 — 01-3
H. Chen

EXAFS, small-angle X-Ray scattering and STEM investigation of nucleation and growth kinetics in devitrifying glass, and associated microstructural and compositional changes.

108. SOLID DIELECTRICS — $ 90,000 — 01-3
D. A. Payne

Synthesis, processing, characterization and property measurements on new and improved polar materials for pyroelectric, ferroelectric and piezoelectric applications in energy conversion and detection systems. Relationship between polycrystalline and single crystal properties. STEM analysis of electrical and mechanical internal boundary conditions in hot pressed, forged and extruded mechanically oriented microstructures.

109. GRAIN GROWTH IN ALUMINA — $ 44,000 — 01-3
D. S. Phillips

STEM investigation of solute drag and pore-grain boundary interaction effects in sintering of doped alumina.

110. HYDROGEN TRAPPING IN BCC ALLOYS — $ 43,000 — 01-3
T. J. Rowland

Atomic and electronic structure of trapping sites in binary substitutional metallic solid solutions and compounds. Hydrogen/deuterium trapping by solute species using NMR, ion probe, and resistance.

111. AMORPHOUS MATERIALS — $ 51,000 — 01-3
H. J. Stapleton

Effects of tunneling states and disorder in fast ionic conductors, doped crystals, and amorphous semiconductors, using electron spin relaxation and double resonance techniques.

112. LOW TEMPERATURE STUDIES OF DEFECT STRUCTURE IN SOLIDS — $ 123,000 — 02-2
A. C. Anderson

Effect of interfaces, lattice defects and disorder on thermal transport at low temperature. Disordered interstitial solutions, solid electrolytes, polymers and hydrogen in metals. Development of low-temperature thermometry.

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (Continued)

113. RESPONSE OF SOLIDS TO ELECTROMAGNETIC RADIATION — $ 85,000 — 02-2
J. D. Dow

Optical semiconductor response to intense light; optical properties of heavily doped semiconductors and model photovoltaic and electroluminescent materials. LEED and photoelectron spectra of layered dichalcogenides. Theory of synchrotron radiation spectra of deep cores in metals. Theory of alloys.

114. USE OF VERY HIGH PRESSURES TO INVESTIGATE THE STRUCTURE OF MATTER — $ 173,000 — 02-2
H. G. Drickamer

Use of very high pressures to investigate phosphor efficiency, energy transfer and photochemistry of inorganic and organic solids and polymers, and to study viscosity effects on luminescence.

115. EXCITON COLLECTION FROM ANTENNA SYSTEMS INTO ACCESSIBLE TRAPS — $ 50,000 — 02-2
L. R. Faulkner

Exciton propagation from absorbing chromophores dispersed in polymer films to trapping sites on film surfaces at monolayer coverage. Controlled molecular assemblies of three dimensional reaction systems.

116. IMPURITIES IN SUPERCONDUCTORS — $ 50,000 — 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.

117. ULTRASONIC INVESTIGATIONS OF THE STRUCTURE OF MATTER — $ 132,000 — 02-2
A. V. Granato

Investigation by ultrasonic methods of impurity - self interstitial interactions in irradiated metals, of hydrogen in bcc metals and of nonlinear mechanical properties of solids.

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (Continued)

118. DEFECT PROPERTIES OF SOLIDS — $ 127,000 — 02-2
D. Lazarus

Atomic mobility in bcc transition metals and in solid electrolytes at high temperature, and high pressure. Spin-glass and mictomagnet properties at high pressure.

119. PROPERTIES OF CRYSTALLINE CONDENSED GASES — $ 107,000 — 02-2
R. O. Simmons

Thermal and isotopic point defects in helium crystals; phase separation in solid helium; phase transitions and elastic properties of solid methanes; quantum effects in diffusion.

120. NUCLEAR MAGNETIC RESONANCE IN SOLIDS — $ 154,000 — 02-2
C. P. Slichter

Investigations of magnetic impurities in nonmagnetic metals, of layered materials with charge density waves and of platinum-silica reforming hydrocarbon catalysts, using nuclear magnetic resonance methods.

121 PHYSICAL PROPERTIES OF CERAMIC MATERIALS — $ 81,000 — 02-2
W. S. Williams

Second phase precipitates and mechanical properties of titanium diboride; influence of hydrogen doping and vacancy ordering on superconducting transition in nonstoichiometric niobium carbide; evaluation of CVD titanium carbide for photothermal conversion of solar radiation.

122. PHYSICAL PROPERTIES OF ORDERED AND DISORDERED SOLID SOLUTIONS — $ 27,000 — 02-2
H. Zabel

X-ray and neutron-scattering studies of structure and phase changes in graphite intercalation compounds and hydrogen-metal systems.

123. RADIATION DAMAGE IN SOLIDS — $ 90,000 — 02-4
J. S. Koehler

Mechanisms of generation and annealing of radiation damage in metals and semiconductors. Structure of point defects; effect of defects on physical properties.

LAWRENCE BERKELEY LABORATORY
University of California
Berkeley, California 94720

Materials and Molecular Research Division
A. W. Searcy - Phone: (FTS) 451-6062, or 415/486-6062

124. ATOMIC RESOLUTION MICROSCOPY — $215,000 — 01-01
R. Gronsky and G. Thomas

Development and application of electron-optical instrumentation and techniques to image atoms in solids. Real-space structural analysis of crystalline and amorphous materials. Identification of atomic mechanisms responsible for solid state reactions, bulk behavior, surface properties and performance of materials used in the energy technologies.

125. MICROSTRUCTURE, PROPERTIES, ALLOY DESIGN: INORGANIC MATERIALS — $475,000 — 01-01
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 and magnetic property improvements - energy conservation; systems under investigation include ferrous alloys, steels, alloys undergoing spinodal and ordering transformations, and ceramics. Quantitative analyses of structure by high resolution electron microscopy, spectroscopy and diffraction and high voltage electron microscopy.

126. 1.5 MeV ELECTRON MICRSCOPE — $320,000 — 01-01
K. H. Westmacott

Crystal lattice defect-solute atom interactions, segregation phenomena, precipitation reactions, structural transitions. High voltage electron microscopes equipped with environmental cells used for dynamic in-situ studies of gas-solid reactions, microstructural stability in hostile environments and mechanisms for improving material performance.

127. THEORETICAL PROBLEMS IN ALLOY DESIGN — $440,000 — 01-02
J. W. Morris, Jr.

Mechanical properties of alloys: quantitative characterization of microstructure. Use of analytic, computer simulation, and experimental techniques. Alloy design: design of new engineering alloys to meet advanced requirements in the energy area.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Reserach Division - (Continued)

128. STRUCTURE-PROPERTY RELATIONSHIPS IN SEMICONDUCTOR MATERIALS — $240,000 — 01-02
J. Washburn

Structural characterization and measurement of properties of materials potentially useful to collection or conversion of solar energy. Point defect clustering, properties of grain boundaries and mechanisms of mass transport in silicon; high resolution transmission electron microscopy. Properties of mixed cadmium-zinc sulfide and zinc diphosphide as possible materials for solar cell use.

129. MECHANICAL PROPERTIES OF CERAMICS — $190,000 — 01-02
A. G. Evans

Study of toughening mechanisms in brittle materials. Investigation of concurrent deformation and failure mechanisms in ceramic polycrystals at elevated temperatures, to relate mechanical properties to microstructure, local chemistry, etc. Investigation of pore removal and grain growth during final stage sintering. The studies involve both modelling and the observation, characterization of microstructural details, microstructural changes, etc., using electron microscopy.

130. SUPERCONDUCTIVITY EFFECTS - HIGH FIELD SUPERCONDUCTIVITY — $130,000 — 01-03
M. Rosen

Application of powder metallurgy techniques and the liquid infiltration process for the preparation of higly flexible superconducting wires of the inherently brittle A-15 compounds; Nb_3Sn, Nb_3(Al-Si), and Nb_3(Al-Ge). Investigation of the diffusional mechanisms controlling the physical and mechanical properties of the A-15 compounds. Determination of the critical superconducting parameters and their behavior as affected by the mode of preparation, strain, and magnetic fields.

131. INTERFACES AND CERAMIC Microstructures — $130,000 — 01-03
J. A. Pask

Kinetics and mechanisms of solid state reactions, nucleation and growth phenomena, and distribution of phases in multiphase ceramic systems; applications to microstructure design of materials whose principal constituents are within the Al_2O_3-SiO_2 system. Thermodynamic considerations of sintering with and without a liquid phase. Mechanisms of corrosion of ceramic materials. Thermodynamics and kinetics of electrochemical reactions at glass-metal and ceramic-metal interfaces.

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

132. HIGH TEMPERATURE REACTIONS $240,000 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 surface kinetics, solid solution thermodynamics, the catalysis of metal sulfate decomposition, the catalysis of gas reactions by solid surfaces.

133. CHEMICAL PROPERTIES OF CERAMIC ALLOYS AND PROCESSING OF CERAMIC MATERIALS $130,000 01-03
L. C. De Jonghe

Mechanisms and kinetics of gas-solid reactions, in particular reactions between oxides and hydrogen; study of these reactions by means of thermogravimetrical analyses and microscope techniques, including high-resolution transmission electron microscopy and analytical scanning transmission electron microscopy. Studies of liquid phase and transient liquid phase sintering; examination of densification kinetics, and micromorphological evolution during sintering with liquid or transient liquid phases.

134. STRUCTURE AND ELECTRICAL PROPERTIES OF COMPOSITE MATERIALS $105,000 01-03
R. H. Bragg

Carbon materials: structure, electrical and thermophysical properties of carbon materials heat treated in the range 1,000°C - 3,000°C. Characterization using X-ray and electron diffraction, small angle scattering, conductivity, Hall Effect and magnetoresistance in magnetic fields to 5.0 Tesla. Measurements in the range 4.2°K - 300°K. Mechanisms of graphitization and point defect annealing in Glassy Carbon and Pyrolytic Graphite. Composition: aligned two phase microstructures obtained by direcitonal solidification of eutectic alloys. Effect of microstructure on electrical, thermophysical and mechanical properties. Usefulness of rule of mixtures as a predictor.

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

135. HIGH TEMPERATURE OXIDATION AND CORROSION OF MATERIALS — $315,000 — 01-03
D. P. Whittle

Determination of the effects of metallurgical and environmental variable on the surface degradation of materials in complex gaseous atmospheres containing sulfur compounds. The chemistry of sulfatic depositions and their influence on metallic corrosion. Mechanisms of degradation, and their relationship to diffusional, structural and compositional parameters of the metal oxides and sulfides involved. Oxide stoichiometry changes in the presence of sulfur. Active element additions to alloys and coatings to promote improved scale/substrate adhesion, and the importance of coating structure; the nature of the scale/substrate interface. Multicomponent diffusion in coating/alloy systems and quantitative relationships to the fundamental thermodynamic and transport properties involved.

136. REFRACTORIES PROJECT: CHEMICAL-MECHANICAL STABILITY — $ 0 — 01-03
L. C. De Jonghe, A. G. Evans, and D. P. Whittle

High-temperature reaction between two-phase refractories and corrosive gases and melts. Densification behavior in presence of liquid and intergranular phases. Creep of porous and of two-phase refractories: chemical-mechanical interaction at high temperatures in the Al_2O_3-CaO system. To start in FY 1981.

137. EROSION-CORROSION WEAR PROGRAM — $400,000 — 01-05
A. V. Levy

Determination of mechanisms of erosion and combined erosion-corrosion of metals, ceramics and coatings and scales on metals in two-phase, solid particle-gas and liquid flows representative of those in coal conversion processes. Investigation of the fluid mechanics of two-phase flow to establish the trajectories of entrained particles in various flow passage geometries. Development of analytical models to define particles trajectories and erosion mechanisms over a wide range of operating conditions. Establishment of material design criteria for erosion-corrosion resistant materials.

138. IN-SITU INVESTIGATION OF GAS-SOLID REACTIONS BY ELECTRON MICROSCOPY — $ 60,000 — 01-05
J. W. Evans and K. H. Westmacott

The investigation of in-situ reactions using an environmental cell in the existing 650 kV electron microscope and the new 1.5 MeV electron microscope. Emphasis is on the investigation of the effect of microstructure on reactions between gases and solids. Nickel oxide reduction by hydrogen has been investigated in ex-situ experiments and will be the first to be studied while reacting in the microscope; subsequently oxidation, sulfidation and other reactions of significance to materials performance in energy conversion systems will be investigated.

LAWRENCE BERKELEY LABORATORIES
Materials and Molecular Research Division - (Continued)

139. FAR INFRARED SPECTROSCOPY $200,000 02-02
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 chemically adsorbed on metal surfaces, the infrared properties of solids with charge-density wave transitions, the far infrared spectra of electrons trapped on the surface of liquid helium, 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.

140 EXPERIMENTAL SOLID STATE PHYSICS AND QUANTUM ELECTRONICS $236,000 02-02
Y. R. Shen

Development of modern optical techniques and their applications to the study of linear and nonlinear optical properties of materials including gases, liquids, liquid crystals, metals, semiconductors, and magnetic crystals. Investigation of the new phenomena of interaction of light with matter and use of lasers to study current problems of interest, such as isotope separation, photochemistry, and surface phenomena.

141. EXCITED QUANTUM FLUIDS IN SOLIDS $152,000 02-02
C. D. Jeffries

Study of phenomena arising when light strikes matter, in particular semiconductors like germanium, at low temperatures: electrons are excited into higher states leaving vacant states, or holes. At sufficient densities, excitons condense into a metallic electron-hole liquid, a novel state of matter. Being studied are: droplet nucleation; surface tension effects; gas-liquid coexistence curves and phase diagrams; kinetics of formation and decay; motion and spatial distribution of free excitons and drops under pulsed and steady excitation; unusual explosive formation kinetics at high excitation; unusual optical hysteresis and optical nonlinearities of the gas-liquid systems, and the possible transient existence of biexcitons and high excitonic molecules during the nucleation of the liquid.

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

142. SUPERCONDUCTIVITY, SUPERCONDUCTING DEVICES, AND 1/f NOISE — $232,000 — 02-02
J. Clarke

Development of Superconducting Quantum Interference Devices (SQUIDS) for measuring small fluctuations in magnetic fields and magnetic field gradients highly reliable and easily operated devices using integrated thin-film technology. Use of SQUIDS in magnetotelluric measurements of the apparent resistivity of the earth's crust; acquisition and analysis of magnetotelluric data. Nonequilibrium superconductivity: enhancement of the superconducting energy gap and transition temperature by microwaves and photons, quasiparticle charge relaxation in presence of magnetic impurities or a supercurrent; response of superconducting films to pulsed perturbations; measurement of the electron-phonon relaxation times in aluminum, tin, and lead.

143. TIME-RESOLVED SPECTROSCOPIES IN SOLIDS — $ 0 — 02-02
P. Y. Yu

Development of an optical system for measuring absorptivity, reflectivity, photoluminescence and light scattering spectra of samples as a function of time with the precision of picoseconds. Phenomena to be studied: relaxation of hot carriers in semiconductors via carrier-phonon interaction; temporal behavior of resonant light scattering spectra; transient optical response in solids exhibiting spatial dispersion effects, and transient phenomena involving defects and impurities in semiconductors. To start in FY 1981.

144. THEORETICAL STUDIES OF THE ELECTRONIC PROPERTIES OF SOLID SURFACES — $ 40,000 — 02-03
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 develope 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).

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

145. THEORETICAL SOLID STATE PHYSICS — $ 60,000 — 02-03
M. L. Cohen

Analytical techniques augmented by computer computations are being used to explore the properties of real materials. Electronic structure of bulk and surface solids are of primary concern, but calculation of cohesive energies, structural phase transitions, phonon spectra, lattice constants, and other structurally related properties are also in progress. Superconducting mechanisms are being examined, and their relation to electronic properties is being explored. The pseudopotential approach is being used in many of the above calculations, and pseudopotential theory itself is being refined.

146. LOW TEMPERATURE PROPERTIES OF MATERIALS — $140,000 — 03-01
N. E. Phillips

General objectives: obtain low-temperature 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, super-fluids, dielectric solids, and magnetic materials. Heat capacity measurements are confined to temperatures below 25K because usually only in that region can various contributions be reliably separated. The temperature scale for the region from 0.06 to 25K is based on ^{3}He and ^{4}He vapor pressure scales, gas thermometry, and extrapolations of magnetic susceptibility thermometers. It is maintained on germanium resistance thermometers. For temperatures from 0.06K to below 1mK nuclear susceptibility and γ-ray anisotropy thermometers will be used as primary thermometers.

147. ELECTROCHEMICAL PROCESSES — $130,000 — 03-01
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 macroprofiles. Gas-electrolyte-electrode interfaces: supersaturation, coalescence, and bubble separation phenomena. Nonaqueous ionizing media: thermodynamic and kinetic properties of electrode reactions which are not feasible in aqueous media.

148. HIGH TEMPERATURE THERMODYNAMICS — $125,000 — 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 use to test and improve chemical models capable of predicting the thermodynamic properties of high-temperature materials.

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

149. CHEMISTRY AND MATERIALS PROBLEMS IN ENERGY PRODUCTION TECHNOLOGIES — $200,000 — 03-03
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 inclusion, and hydrogen solubility; molecular beam studies of gas-solid reactions, including hydrogen atom reaction with ceramic oxides and refractory carbides and the silane cracking reaction, and radiation-enhanced stress corrosion cracking of zircaloy.

150. PLASMA ENHANCED DEPOSITION OF THIN FILMS — $ 50,000 — 03-03
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 porcesses as they affect solar cell fabrication, integrated circuit processing, magnetic film properties, and structure-property relationships in catalyst support materials.

151. ELECTROCHEMICAL PHASE BOUNDARIES — $145,000 — 03-03
R. H. Muller

Investigation of the formation of boundary layers and thin films at electrochemical interfaces. Solid and liquid films at electrodes; mechanisms of formation, effect on electrochemical reactions, control of film properties. Study of electrochemical processes at high current densities; new means to accelerate electrochemical mass transport; increase of space-time yield, material- and energy-efficiency. Development and use of new optical techniques for the observation of electrode surfaces in liquid media.

152. SOLID STATE AND SURFACE REACTIONS — $300,000 — 03-03
G. A. Somorjai

Studies of catalyzed surface reactions and of the atomic structure and chemical composition of solid surfaces and adsorbed monolayers. Kinetics and mechanisms of catalytic surface reactions on crystal surfaces at low and at high pressures. A combination of surface techniques is used: Auger electron spectroscopy, low energy electron diffraction, electron energy loss spectroscopy, molecular beam scattering, gas chromatography, and mass spectroscopy.

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

153. NUCLEAR MAGNETIC RESONANCE $130,000 03-03
A. Pines

Nuclear spin interactions and their use in developing new nmr techniques. Molecular properties of ordered condensed phases and effect of nuclear spin on chemical processes. Development of the concept of coherent multiple quantum nmr and its use for the analysis of oriented materials. Molecular behavior of organized matter, this includes fuel material, liquid crystals, molecules adsorbed on surfaces and molecules excited by light.

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

G. Dorough - Phone: (FTS) 532-4892 or 415-422-4892
L. Roberts - Phone: (FTS) 532-6369 or 415-422-6369

154. HOT CORROSION STUDIES RELATED TO FOSSIL FUELS — $250,000 — 01-1
J. Truhan

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

155. RAPIDLY QUENCHED AMORPHOUS MATERIALS RESEARCH — $100,000 — 01-3
B. Holt, C. Cline

Synthesis of amorphous, metastable crystalline, or supersaturated solid solutions of beryllium-containing alloys by rapid quench techniques. New materials include Beta-beryllium stabilized at room temperature and the extended solid solution of beryllium in aluminum. Mechanical property measurement and structural analysis for evaluation of potential technological applications.

156. LOW-INDEX OPTICAL MATERIALS RESEARCH — $235,000 — 02-2
M. Weber, A. Rosencwaig, C. Cline

Nonlinear optical properties of transparent materials subject to intense light beams; intensity-dependent refractive index change and two-photon absorption at near-ultraviolet to near-infrared wavelengths. Time-resolved laser interferometry used to measure nonlinear refractive index. Materials include glasses (fluorides, oxides) and crystals (alkali and alkaline-earth halides, oxides).

LAWRENCE LIVERMORE NATIONAL LABORATORY (continued)

157. LASER-EXCITED FLUORESCENCE IN AMORPHOUS SOLIDS — $220,000 — 02-02
S. Brawer, M. Weber

Laser-induced fluorescence line narrowing and site selection spectroscopy to probe variations in local fields and electron-phonon coupling 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.

158. SURFACE PHYSICS AND CHEMISTRY OF LASER INDUCED DAMAGE — $235,000 — 02-2
W. Lowdermilk, W. Siekhaus

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 of atomically exposed surfaces, dependence of damage thresholds on the physical structure of surfaces, effects of absorption of foreign atoms, surface chemical reactions, and migration of impurities. Crystalline and amorphous samples are prepared in a vacuum chamber and tested in situ using 1 μm laser pulses. Photon induced desorption is monitored by mass spectrometry and Auger analysis.

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

We have measured D_2+T_2 chemical reaction rates in the solid and liquid phases by infrared spectroscopy. We are currently measuring D_2-T_2 rotational reaction rates by nuclear magnetic resonance. We have completed engineering-type measurements on a DT-He^3 mixture phenomenon that halts the flow of gas into the cryostat. The D_2+T_2 gas phase kinetic experiment using mass spectroscopy is ready to run. The solid thermal conductivity cell is under construction.

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

Chemistry - Material Science Division
W. J. Maraman - Phone: (FTS) 843-4563 or 505-667-4563

160. THE EFFECT OF SELF-IRRADIATION ON STABILITY OF SIMULATED CERAMIC NUCLEAR WASTE — $125,000 — 01-4
F. W. Clinard, Jr., C. C. Land, D. E. Peterson, D. L. Rohr, R. B. Roof

Alpha decay self-damage in the zirconolite phase of SYNROC; fabrication and characterization; doping with $^{238}PuO_2$; density, strength, fracture behavior, thermal conductivity, x-ray crystal structure, and microstructural changes after aging. Spontaneous fragmentation of alpha-active $^{238}PuO_2$; weight loss, particle size and morphology, electron microscopy; effect of environment and fabrication parameters; mechanism(s) responsible; relationship to stability of nuclear waste.

161. RADIATION EFFECTS STUDIES FOR ADVANCED ENERGY TECHNOLOGIES — $375,000 — 01-4
D. M. Parkin, J. R. Cost, W. F. Sommer

800 MeV proton (LAMPF) irradiation of Al under cyclic stressing and proton irradiation effects in technologically important materials; interaction of radiation damage and mechanical damage; modeling of damage microstructure development under pulsed irradiation; investigation of the WNR facility for radiation effects studies; radiation effects in amorphous metals; atomic mobility in amorphous and crystalline metals; application of computer image enhancement techniques to the analysis of void micrographs.

162. HIGH TEMPERATURE MATERIALS FOR ENERGY APPLICATIONS — $100,000 — 01-3
E. K. Storms

Mass spectrometric vapor pressure measurements to determine surface composition of freely vaporizing materials; thermionic work function measured and related for the first time to the emitting surface composition; information used to calculate thermodynamic properties, phase boundaries, and relationship to electron energy levels as a function of stoichiometry and temperature; work has involved LaB_6, NdB_6, GdB_4 and the Mo-B system; applications to thermionic energy conversion and intense electron source design.

LOS ALAMOS SCIENTIFIC LABORATORY

163. MATERIAL DEFORMATION UNDER MULTIAXIAL LOADING — $250,000 — 01-5
S. S. Hecker, J. J. Petrovic
M. Stout, K. Staudhammer
D. L. Rohr

Multiaxial deformation of aluminum, aluminum alloys, brass and 304 stainless steel; biaxial tube testing; yield surfaces and stress-strain relations under multiaxial loading; evolution of dislocation substructure with strain, strain state and strain rate; deformation-induced transformation in 304 stainless steel; brittle fracture of Al_2O_3 under multiaxial stresses; Weibul brittle fracture theory; fracture toughness of ceramics.

164. CTR RELATED TRITIUM CHEMISTRY RESEARCH ASSOCIATED WITH THE BREEDER BLANKET AND CONTAINER MATERIALS — $170,000 — 03-2
J. L. Anderson, D. H. W. Carstens

Equilibrium pressure measurements of tritium, deuterium, protium, and mixtures of these isotopes over lanthanides and low melting point lanthanide alloy eutectics (gettering material); studies of the removal of tritium by gettering materials from helium streams as a function of flow rate and temperature in the PPM range of tritium; solubility of container materials in the low melting point gettering alloys.

Physics Division
G. A. Keyworth - Phone: (FTS) 843-4117 or 505-667-4117

165. MATERIALS RESEARCH ON THE LOS ALAMOS SPALLATION NEUTRON SOURCE — $620,000 — 02-1
R. Silver, J. Yarnell, P. Seeger,
T. A. Kitchens, J. Eckert

Materials research and the development of instrumentation to utilize the special characteristics of the new pulsed spallation neutron source at Los Alamos. Inelastic neutron scattering studies of metal hydrides, chemical spectroscopy and surface studies. Structural studies by neutron diffraction of molecular liquids, powders, amorphous materials, and single crystals. Development of time of flight instrumentation unique to spallation sources.

LOS ALAMOS SCIENTIFIC LABORATORY

166. ULTRAHIGH-PRESSURE STUDIES OF HYDROGEN — $150,000 — 02-2
R. L. Mills, D. H. Liebenberg

Measure simultaneously P, V, T, and ultrasonic velocity of cryogenic gases and their mixtures to 40 kbar in a piston-cylinder apparatus to determine consistent equations of state (EOS); carry out measurements of Brillouin, Raman, and x-ray scattering on condensed gases and mixtures to 500 kbar in diamond anvil cells (DACs) to study EOS, phase changes, and molecular interactions; study superconducting and insulator-metal transitions on samples under hydrostatic helium pressures to 500 kbar in DACs; develop multistage systems that combine DACs with other pressure devices to reach 1 Mbar in the hydrogen isotopes.

Theoretical Division
George I. Bell - Phone: (FTS) 843-4401 or 505-667-4401

167. ELASTIC WAVE SCATTERING AND QUANTITATIVE FLAW IDENTIFICATION — $150,000 — 01-5
J. E. Gubernatis
W. M. Visscher

Development of an analytical scientific reference data base for flaw identification calculations of scattering phenomena selected as representative of applications; study will use an integral equation method, the method of optimized truncation, and Padé approximants; scattering will be calculated for special geometries by various approximations and compared with exact results from a sphere and a circular crack; single scattering results will be used in development of multiple scattering theories.

168. LOS ALAMOS EQUATION OF STATE LIBRARY — $254,000 — 02-3
G.I. Kerley, B.I. Bennett,
J.D. Johnson, R.C. Albers,
S. P. Lyon, and J. Abdallah

Maintain a computer-based library of equations of state (EOS) and other material properties for application to energy programs. Survey current user requirements for the EOS and calculate or acquire and evaluate the needed data. Store EOS data in tabular form suitable for use in realistic hydrodynamic code calculations and other applications. Distribute data to users on magnetic tape 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.

MOUND LABORATORY
P. O. Box 32
Miamisburg, Ohio 45342

W. H. Smith - Phone: (FTS) 774-7296 or (513) 866-7296

169. SOLAR THERMAL ENERGY MATERIALS $250,000 01-3
L. J. Wittenberg

Advanced materials studies at elevated temperatures of potentially improved components of liquid heat transfer systems for solar energy utilization by photothermal processes; identification of soluble chromophoric materials dissolved in fluids which are liquid at ambient temperature but useful to 300°C; long term photothermal stabilities; specific heat, density, viscosity, thermal diffusivity; spectral and physical properties of fused salts containing selected chromophores for potential use above 500°C; thermal energy storage materials for use in the 100-300°C range including phase change materials; optical properties of thin film liquid metals.

OAK RIDGE ASSOCIATED UNIVERSITIES
P. O. Box 17
Oak Ridge, Tennessee 37830

William E. Felling - Phone: (FTS) 626-3304 or (615) 576-3304

170. DOE FACILITY USERS PROGRAM $ 80,000 01-1
W. E. Felling

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

171. THEORETICAL STUDIES OF METALS AND ALLOYS $360,000 01-1
J. S. Faulkner, W. H. Butler, G. S. Painter, G. M. Stocks, F. W. Averill, A. T. Fromhold, F. J. Pinski

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 CPA treatment of random substitutional solid solutions, comparison with results of photoemission experiments, extension of theory beyond CPA; calculation of binding energies and phase stability in alloys; superconducting transition temperature and H_{C_2} and phonon line width; phonon contribution to lattice conduction in metals; electron-phonon and electron-electron enhancement effects in metals.

172. X-RAY SCATTERING RESEARCH $135,000 01-1
B. S. Borie, R. W. Hendricks

Small-angle x-ray scattering from voids in neutron and ion irradiated metals; structure of polymers, effect of stress and transformations; coal and oil shale; theoretical and experimental studies of extinction phenomena; crystallography of modulated structures.

173. HIGH-TEMPERATURE STRUCTURAL CERAMICS $560,000 01-1
V. J. Tennery, C. B. Finch, G. W. Clark, J. D. Holder, C. S. Yust, O. C. Kopp

Synthesis, fabrication, characterization, and evaluation of hard structural ceramics including materials from TiB_2-Ni, TiB_2-CrB_2-Ni, other boride and carbide systems with objective of determining compositional and microstructural requirements for severe erosive and corrosive environments; preparation and evaluation of directionally solidified eutectics in $ZrO_2(Y_2O_3)$-$Al_2O_3(Cr_2O_3)$-Mo and related systems as tool materials and grinding media; mechanisms for increasing fracture energy and high-temperature strength of selected oxide and carbide structural ceramics.

174. STRUCTURE OF COAL $135,000 01-1
L. A. Harris, C. S. Yust

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.

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

175. X-RAY RESEARCH USING SYNCHROTRON SOURCES — $185,000 — 01-1
C. J. Sparks, H. L. Yakel, G. E. Ice

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.

176. HIGH VOLTAGE AND ANALYTICAL ELECTRON MICROSCOPY — $275,000 — 01-1
R. W. Carpenter, J. Bentley, E. A. Kenik

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.

177. DEFORMATION AND MECHANICAL BEHAVIOR OF STRUCTURAL MATERIALS — $450,000 — 01-2
M. H. Yoo, K. Farrell, R. A. Vandermeer, C. L. White, J. C. Ogle

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; anelastic recovery within grains; hydrogen in these alloys; segregation of impurities to grain boundaries and creep cavities; dynamic recrystallization; small-angle neutron scattering studies of cavity growth during creep and fatigue.

178. KINETICS AND MECHANISMS OF SURFACE AND SOLID STATE REACTIONS — $595,000 — 01-3
J. V. Cathcart, R. E. Druschel, R. A. McKee, R. E. Pawel, G. F. Petersen

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. Theoretical treatment of vacancy and interstitial diffusion in compounds having high defect concentrations.

179. PHYSICAL PROPERTIES RESEARCH — $325,000 — 01-3
D. L. McElroy, J. P. Moore, R. K. Williams

Development and application of measurement methods for physical property studies from 4.2 to 2600K; 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, Cr); phonon-phonon scattering in insulating solids, effect of cation-anion mass ratio, grain boundaries and crystal structure; properties of LRO alloys.

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

180. AMORPHOUS AND METASTABLE MATERIALS $430,000 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 and fluxoid pinning in amorphous superconductors; 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.

181. RADIATION EFFECTS $1,250,000 01-4
L. K. Mansur, W. A. Coghlan, K. Farrell, E. A. Kenik, M. B. Lewis, N. H. Packan, T. C. Reiley

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; irradiation creep simulation using ORIC and neutron pre-irradiated specimens; creep of pressurized tubes in EBR-II; 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.

182. EROSION AND WEAR OF CERAMICS $ 90,000 01-5
C. S. Yust

TEM and SEM studies of single particle impacts on polycrystalline alumina and single crystal Al_2O_3 and LiF; dislocation arrangements in subsurface volume; friction and microstructural changes caused by sliding wear; effects of temperature, atmosphere, crystal orientation, strength and deformation mechanisms; erosion and wear of metallic bonded borides; effects of high deformation rates on structure.

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

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

184. STUDIES IN NONDESTRUCTIVE EVALUATION $100,000 01-5
R. W. McClung, W. A. Simpson

Theoretical and experimental study of acoustic wave systems interacting with internal boundaries in solids, reflection, diffraction and refraction of waves at weld-base metal interfaces; study of second-order effects on eddy-current propagation to describe absolutely flaw size and shape.

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

185. INTERATOMIC INTERACTIONS IN CONDENSED SYSTEMS — $1,205,000 — 02-1
R. M. Nicklow, J. W. Cable, A. M. Castets, H. R. Child, B. Hennion, W. C. Koehler, B. Lebech, H. A. Mook, R. M. Moon, Y. Noda, R. E. Parra, H. G. Smith, Y. Tsunoda, N. Wakabayashi, S. A. 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 $LaSn_3$, SmS, and martensitic alloys; magnetic excitations in $HoCo_2$, $HoFe_2$, Fe-Al alloys, Gd at high temperatures, and Er; magnetic structures of Nd and $CeAl_2$; magnetic form factors of mixed valence materials; structures of composition modulated systems.

186. PROPERTIES OF DEFECTS, SUPERCONDUCTORS AND HYDRIDES — $705,000 — 02-1
R. M. Moon, J. W. Cable, H. R. Child, W. C. Koehler, H. A. Mook, R. M. Nicklow, H. G. Smith, S. Spooner, N. Wakabayashi, G. D. Wignall, G. Zaccai

Elastic, inelastic and small-angle scattering of neutrons by superconductors, metal hydrides, and defects in single crystals; lattice dynamics of α-U, A15 compounds, PbF_2, AgBr, AgI; defects in KCl and CaO; proton diffusion in biological systems; magnetic structures in reentrant superconductors; SANS from coal solutions, oil shale, polymer blends, and NbH_x.

187. PHYSICAL PROPERTIES OF CERAMICS — $310,000 — 02-2
E. Sonder, Y. Chen, N. J. Dudney, J. Gastineau, F. A. Modine, R. A. Weeks

Solid state reactions at high temperatures involving charge and mass transport, defect structures, and valence changes of impurities in materials such as MgO, Al_2O_3, and $MgAl_2O_4$; effects of impurities, dislocations, and ambient oxygen pressure on electric conduction and other physical properties; determination of the mechanisms involved in accelerated electrical breakdown at high temperatures under moderate electric fields; techniques include measurements of electrical conductivity and dielectric constant, thermoelectric power, diffusion coefficients, optical spectroscopy, electron paramagnetic resonance, and electron microscopy.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

188. HIGH TEMPERATURE PROPERTIES OF CARBIDES AND NITRIDES — $165,000 — 02-2
F. A. Modine, G. R. Gruzalski

Intrinsic and defect controlled properties of transition metal carbide and nitride single crystals; stoichiometry, perfection and impurity content of selected specimens determined by x-ray, optical, and other analytical techniques; information about electronic structure obtained from optical properties; defects investigated by x-ray scattering and transmission electron microscopy; charge and mass transport properties of the materials correlated with stoichiometry, defects, and electronic structure.

189. SOLID ELECTROLYTES AND SUPERIONIC CONDUCTIVITY — $305,000 — 02-2
J. B. Bates, G. M. Brown,
W. E. Brundage, N. J. Dudney,
H. L. Engstrom, B. C. Larson,
J. C. Wang

Mechanisms of high ionic conductivity in the beta- and beta"-aluminas; effects of impurities and crystal growth conditions on conductivity; effect of water intercalation on ion transport in the beta- and beta"-aluminas; thermodynamics and kinetics of water intercalation; 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.

190. PHYSICAL PROPERTIES OF SUPERCONDUCTORS — $420,000 — 02-2
S. T. Sekula, B. R. Appleton,
D. K. Christen, H. R. Kerchner,
B. W. Stritzker, 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-

191. PREPARATION AND CHARACTERIZATION OF RESEARCH MATERIALS — $700,000 — 02-2
L. A. Boatner, G. C. Battle, W. E. Brundage, Y. K. Chang, T. F. Connolly, G. R. Gruzalski

Growth and characterization of high-quality single crystals of metals, alloys, and insulators; 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); flux growth of single crystals of fast-ion conductors (β-alumina, β"-alumina); 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; 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 the electron-beam float-zone technique; compilation and dissemination of information on the physical properties and availability of single crystals and research materials by the Research Materials Information Center.

192. PHOTOPHYSICAL PROCESSES OF SOLAR ENERGY CONVERSION — $615,000 — 02-2
R. F. Wood, J. W. Cleland, H. L. Engstrom, L. S. Darken, J. Fletcher, M. Lu, G. E. Jellison, B. C. Larson, D. H. Lowndes, J. Narayan, R. D. Westbrook, C. W. White, R. T. Young

Effects of point defects, defect clusters, dislocations, grain boundaries, stacking faults, and chemical impurities on electrical and optical properties of single crystal and polycrystalline Si; thermal neutron transmutation, diffusion, and ion implantation doping experiments for fabrication of p-n junctions; fabrication of high efficiency Si and GaAs 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 Raman spectroscopy), transmission electron microscopy, electron paramagnetic resonance, x-ray scattering, surface photovoltage, secondary ion mass spectrometry, and Rutherford ion backscattering property measurements; grain boundary compensation in polycrystalline Si; 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; grain growth in polycrystalline materials; graphoepitaxy; chemical vapor deposition on low-cost substrates.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

193. FUNDAMENTAL ASPECTS OF METAL FRACTURE $285,000 02-2
S. M. Ohr, S.-J. Chang,
S. Kobayashi, J. Narayan,
T. S. Noggle

Theoretical and experimental 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; distribution of dislocations in the plastic zone ahead of the crack tip in metals and ceramics; dislocation theory of J-integral; theory of the plastic zone with a dislocation-free zone.

194. THEORY OF CONDENSED MATTER $900,000 02-3
R. F. Wood, J. H. Barrett,
J. A. Blackman, W. L. Clinton,
J. F. Cooke, H. L. Davis,
L. J. Gray, T. Kaplan,
M. E. Mostoller, O. S. Oen,
A. K. Rajagopal, M. Rasolt,
M. T. Robinson, M. V. K. Ulehla,
J. C. Wang

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; electron screening and phonon spectra; lattice dynamics of high T_c superconductors; 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.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

195. LOW TEMPERATURE RADIATION EFFECTS — $350,000 — 02-4
R. R. Coltman, Jr., C. E. Klabunde, J. M. Williams

Fission-neutron damage rates at 4.7 K for damage-efficiency determinations; magnetoresistance of irradiated Cu for composite superconductors; defect-production studies in pure and doped metals fast-neutron irradiated near room temperature; effects on insulators for superconducting magnets irradiated at 4.7 K; effect of fission-neutron irradiation at 4.7 K on the transition temperature of Pd films; stored energy in ^{10}B and ^{235}U fission-fragment-damaged Cu.

196. X-RAY DIFFRACTION AND ELECTRON MICROSCOPY — $415,000 — 02-4
T. S. Noggle, J. F. Barhorst, B. C. Larson, J. Narayan, S. M. Ohr, J. Fletcher

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; 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.

197. NORMALIZATION OF ION AND NEUTRON DAMAGE — $180,000 — 02-4
T. S. Noggle, B. R. Appleton, O. S. Oen, D. B. Poker, J. M. Williams

Normalization of damage production rates using fission neutrons and MeV Ni ion irradiation of thin films of Ni and Fe-Ni-Cr alloys; damage production rates as a function of ion penetration depth for Ni ions in Ni and stainless steel; damage theory computations.

198. GASES IN METALS — $95,000 — 02-4
D. B. Poker, J. M. Williams

Interactions of light gas atoms with defects in metals; diffusivity of He in Ni and stainless steels at high temperatures with and without radiation-produced defects; diffusion of interstitial He at low temperatures; symmetries and binding energies of H and He with point defects, defect clusters, and dislocations in Nb and Pd; techniques include gas-evolution studies, ultrasonic internal friction, ion implantation, and reactor neutron irradiation.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

199. SURFACE PHYSICS AND CATALYSIS $620,000 02-5
L. H. Jenkins, H. L. Davis,
H. C. Eaton, R. W. Johnson,
M. E. Mostoller, J. R. Noonan,
S. Overbury, M. Rasolt,
M. V. K. Ulehla, G.-C. Wang,
J. F. Wendelken, C. W. White,
D. M. Zehner

Studies of the 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), low energy ion scattering spectroscopy (ISS), polarized low energy electron diffraction (PLEED), photoemission, and computer simulations for surface crystallography studies; LEED 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; 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.

200. ION BEAM ANALYSIS AND ION IMPLANTATION $650,000 02-5
B. R. Appleton, J. H. Barrett,
Y. K. Chang, O. W. Holland,
O. A. Meyer, J. Narayan,
T. S. Noggle, P. P. Pronko,
O. E. Schow III, S. T. Sekula,
B. W. Stritzker, N. G. Thompson,
C. W. White, J. M. Williams,
S. R. Wilson, S. P. Withrow,
D. M. Zehner

Continued development of positive ion crystallography of surfaces (PICS) technique for surface studies; surface investigations of pulsed laser processed Si, Ge, and GaAs single crystals; determination of the lattice sites of B, As, Sb, In, Bi, Ga, Cu, Fe, Zn, and Al in ion-implanted, laser-annealed Si single crystals; discovery and investigation of enhanced ion scattering yields for H and He ions backscattered 180° ± 0.5° from Al, Si, Cu, Ge, Mo, Ag, Pt, Au, and $Nb_{40}Ni_{60}$ polycrystalline and amorphous targets; development of enhanced backscattering yields for PICS surface studies; resonant nuclear reaction analyses of H, C and F in amorphous Si and coal. Capability for in situ ultra high vacuum ion implantation, ion scattering-channeling and surface analyses, and laser annealing; studies of supersaturated surface alloy formation by laser processing of ion-implanted semiconductors and metals; effect of ion implantation on corrosion mechanisms; alteration of superconducting properties by ion implantation doping and laser processing of superconducting materials; investigations of metastable materials prepared by ion implantation doping and laser processing; ion-implanted and laser-annealed metals; rapid heating and cooling studies; crystal regrowth and solidification phenomena; ion beam and pulsed laser induced materials interactions.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

201. RADIOACTIVE WASTE STORAGE $280,000 02-5
L. A. Boatner, M. M. Abraham
M. Rappaz, P. G. Huray,
C. B. Finch, R. J. Floran

Evaluation of lanthanide orthophosphates as primary containment forms for α-active actinide wastes; growth of actinide doped single crystals; 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 under various conditions; use of a molten urea process for the production of orthophosphate powders with controlled particle sizes; compaction and microstructural characterization of hot-pressed or cold-pressed, sintered orthophosphate bodies; studies of α-particle induced radiation effects in lanthanide orthophosphate compounds.

202. RESEARCH AND DEVELOPMENT - ISOTOPE RESEARCH MATERIALS PREPARATION $300,000 02-5
E. H. Kobisk, W. S. Aaron,
H. L. Adair, D. Frischke,
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, sintering, electrodeposition, molecular plating, zone refining, inorganic chemical methods; characterization of prepared research samples includes x-ray and electron diffraction, electron microscopy (TEM and SEM), microprobe studies, 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

203. CHEMICAL STRUCTURE OF ENERGY RELATED MATERIALS — $840,000 — 03-1

W. R. Busing, G. M. Brown, G. J. Bunick, C. K. Johnson, E. Johnson, A. H. Narten, W. E. Thiessen, R. Triolo

Atomic and molecular arrangements in crystals and in liquids determined by neutron and x-ray diffraction studies; separation of atom-atom pair correlation functions for liquids; small-angle neutron scattering; development of synchrotron radiation facilities. Advancement of computational methods for solving and refining crystal structures; dynamic corrections to neutron scattering intensities; improvement of statistical mechanics for understanding molecular fluids and for extrapolating their physical properties; use of intermolecular potentials to interpret the conformation of molecules in crystals and liquids; development of a graphics display for presenting structures. Materials studied include molten salt catalysts for coal liquefaction, liquid coal extracts, catalysts for the photochemical production of hydrogen, hydrocarbon liquids and liquid mixtures related to petroleum production, micelle-forming liquids, and superionic electrical conductors for storage batteries and fuel cells.

204. HIGH TEMPERATURE CHEMISTRY AND THERMODYNAMICS OF STRUCTURAL MATERIALS — $560,000 — 03-2

J. T. Bell, H. F. Bittner, J. Brynestad, J. D. Redman, G. M. Begun

Chemistry and thermodynamics of structural materials in the 400 to 1000°C range are investigated; reactions, kinetics and thermodynamics describing sorption, corrosion and microphase formation are the primary objectives. Hydrogen isotope sorption by both pure metals and alloys; measurements of tritium permeation rates through structural alloys into steam atmospheres; the effects of surface oxidation on the overall permeation process; and chemical and physical characterization of oxides. Amounts and compositions of the oxides formed by steam oxidation of a given alloy depend on the composition of the alloy, the thermodynamic stabilities of the component metal oxides, the oxidation temperature, the type of surface pretreatment, and the bulk annealing conditions. Another major effort is the investigation of the thermodynamics and kinetics of formation and dissolution of carbide and nitride microphase precipitates.

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

205. PHYSICAL CHEMISTRY OF MOLTEN SALTS IN ENERGY UTILIZATION — $211,000 — 03-3
J. Braunstein, C. E. Vallet

Electrochemical measurements, thermodynamics of irreversible processes, and nuclear magnetic resonance are used to investigate diffusion, migration, electrical conductance, and relaxation in ionic systems such as molten salts, hydrous melts, vitreous and solid electrolytes including fast ion conductors; modelling and measurement of polarization and mass transport in electrolytes and electrodes relevant to high temperature battery and fuel cell applications.

206. LOCALIZED CORROSION AND STRESS CRACKING PHENOMENA RELATED TO ENERGY TECHNOLOGIES — $399,000 — 03-3
F. A. Posey, A. L. Bacarella, G. M. Brown, E. J. Kelly, A. A. Palko

Basic electrochemical investigations of mechanisms of corrosion reactions applicable to localized attack of metals (e.g., titanium, stainless steel) needed for understanding corrosion in active and passive states and effects of restrictive geometries (pitting, crevice corrosion, stress corrosion cracking); kinetics of coupled active-passive electrode systems; speciation effects and kinetics of corrosion reactions in concentrated aqueous electrolytes; development of rapid electrochemical methods for testing susceptibility to localized attack; application of ion implantation techniques to corrosion amelioration and control.

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

207. THERMODYNAMICS OF ENERGY RELATED SYSTEMS — $213,000 — 03-2
T. B. Lindemer, E. C. Beahm, T. M. Besmann

Fundamental chemical thermodynamics studies associated with advanced fast breeder reactor fuels. Basic chemical compatibility of uranium carbides and plutonium carbides with Cr-Fe-Ni alloys. Thermodynamics properties and compounds in the systems U-C-Cr-Fe-Ni and U-Pu-C-Ni. Phase equilibria and thermodynamic properties of the systems $U(C,O)_{1.9}$-C; $U(C,O)_{1.9}$-U(C,O); ThC_2-Th(C,O); $PuO_{1.5}$-$PuC_{1.5}$-Pu(C,O); ThO_2-ThC_2-Th(C,O); ThC_2-Th(C,O); (U,Pu)(C,O)-$(U,Pu)C_{1.5}$; and $(U,Pu)O_2$-$(U,Pu)C_{1.5}$-C.

208. CHEMICAL ENGINEERING RESEARCH — $220,000 — 03-2
J. S. Watson, R. E. Barker, S. D. Clinton

Fundamental measurement and evaluation of material properties and behavior important to chemical processes; the development and evaluation of techniques for characterization and physical removal of solid materials from viscous fluids (e.g., coal-derived liquids). Present efforts focus on studies of electrostatically enhanced deep-bed filtration techniques for removing very small (submicron) solid materials from fluids.

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

S. D. Dahlgren - Phone (FTS) 444-0120 or 509-375-0120

209. METAL-INSULATOR-SEMICONDUCTOR PHOTOVOLTAICS — $115,000 — 01-1
J. E. Garnier, L. C. Olsen

Photoelectric and physical/chemical structure evaluation of MIS photovoltaic cells. Improve understanding of basic parameters which control photovoltaic processes in MIS cells through correlation of device performance to thin film structure/fabrication parameters/ theory. Conduct photoresponse, I-V, C-V, sheet resistance, solar cell efficiency, and optical property measurements. Auger and ESCA surface analysis techniques and ellipsometry used to characterize physical structure of MIS cells. Current efforts devoted to Al-Si and Au-Si single crystal silicon cells.

210. PHOTOELECTROCHEMICAL PROPERTIES OF SOLAR MATERIALS — $85,000 — 01-1
R. Wang

Effects of crystal structure, microstructure, and composition on the photoelectrochemical behavior of semiconductors in liquid electrolyte. Characterization of surface and interfacial structures and properties; bandgap, photoresponse, flatband potential and electrical properties of semiconducting oxides, sulfides, and selenides; crystalline and amorphous Fe_2O_3-TiO_2 phases, MoS_2, TiS_2 and $(TiTa)S_2$ films prepared by high rate sputter deposition, and by electrodeposition; electronic properties and stability of semiconducting films grown on amorphous alloy surfaces; degradation and corrosion of photoelectrodes; and surface modification for enhanced stability and efficiency.

211. SPUTTER-DEPOSITED AMORPHOUS SILICON FOR SOLAR APPLICATIONS — $80,000 — 01-1
P. M. Martin and W. T. Pawlewicz

Investigate the influence of H content and Si-H bonding on optical and electrical properties of sputter-deposited a-Si:H. Investigate the structure and properties of triode-sputtered a-Si:H, plasma energy and deposition rate, kinetics of Si-H reaction in plasma and film, and application of a-Si to thin film optical coatings and multilayer stacks; optical and IR spectroscopic techniques; electrical transport measurements; gas evolution analysis; photoconductivity; XRF; x-ray diffraction.

PACIFIC NORTHWEST LABORATORY (continued)

212. EFFECT OF COAL MICROSTRUCTURE ON PROPERTIES $70,000 01-1
J. M. Lytle and J. L. Daniel

Characterization of coals and subsequent coal grinding products for size, morphology, and composition, including controlled grinding experiments at selected temperature and pressure conditions. Correlate characteristics with physical and mechanical properties. Relate grinding fracture characteristics to microstructure by in-electron microscope dynamic fracture experiments.

213. FUNDAMENTAL STUDIES OF STRESS CORROSION FATIGUE MECHANISMS $190,000 01-2
R. H. Jones, M. T. Thomas, S. M. Bruemmer, D. R. Baer

Investigations of the mechanisms controlling stress corrosion cracking and corrosion fatigue cracking of iron, iron-chromium-nickel and nickel-based alloys in gaseous and aqueous environments. Computer modeling and experimental measurement 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, and crack growth rate of Fe and Ni in aqueous solutions are being studied. 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.

214. OXIDATION AND CORROSION RESISTANT FINE-GRAINED MATERIALS $100,000 01-3
J. T. Prater and D. R. Baer

Investigation of the mechanisms controlling the oxidation and corrosion of sputter-deposited fine-grained and amorphous materials. Relationship of properties to microstructure. High temperature oxidation and sulfidation of stainless steels and Ni-Cr-Al alloys; determine the effect that grain size, stress, and the addition of oxide dispersants and rare earth elements have on oxide adherence; AES, XPS, and nuclear microprobe examination of the diffusion of elements to the surface during protective oxide formation; the mechanism by which sulfur leads to oxide scale deterioration in H_2S, SO_2, and Na_2SO_4 environments. Aqueous corrosion studies of amorphous intermetallic alloys with compositions that afford excellent thermal stability.

PACIFIC NORTHWEST LABORATORY (continued)

215. LEACHING OF GLASS AND CERAMICS $70,000 01-3
G. L. McVay and L. R. Pederson

Investigation of mechanisms of glass and crystalline ceramic interactions with aqueous solutions. Research areas include: surface potential measurements, radioactive tracer diffusion measurements in the bulk material and in the reaction layer, isotopic water reactions coupled with Rutherford backscattering, resorption kinetics, solution analyses, and surface and near surface analyses using ESCA and SIMS coupled with ion milling. Development of a predictive model for leaching.

216. RADIATION EFFECTS ON METALS $465,000 01-4
J. L. Brimhall, E. P. Simonen, H. E. Kissinger, L. A. Charlot, C. H. Henager, Jr., E. R. Bradley

Study of the production, migration, and interaction of radiation produced defects; effect of helium on damage microstructures; dual beam (heavy ion + helium) irradiations; pulsed irradiations; comparison of ion and neutron irradiated microstructures; pure refractory metals, refractory alloys, nickel alloys; stability of amorphous materials under irradiation; use of transmission electron microscopy, resistivity, x-ray diffraction techniques; theoretical analysis of nucleation and growth of defect structures; testing of theoretical models by experiment; studies of radiation enhanced creep by light ions; creep behavior under pulsed irradiation; creep of reactor preconditioned specimens; modeling of creep behavior; transmission electron microscopy of irradiation creep microstructures.

217. RADIATION DAMAGE IN CERAMICS $105,000 01-4
W. J. Weber and R. P. Turcotte

Experimental evaluation of the effects of particle-induced radiation damage on the structure of ceramics. Studies emphasize external alpha bombardment from actinide sources or alpha-recoil damage from internal alpha decay in actinide doped compounds. X-ray diffraction, density, and electron microscopy methods are utilized to study damage ingrowth and annealing kinetics. Emphasis on cubic oxides and halides, amorphization in rare-earth silicates, and testing of theoretical models.

PACIFIC NORTHWEST LABORATORY (continued)

218. SPUTTERING PARAMETER INFLUENCES ON MATERIALS STRUCTURE AND BEHAVIOR — $170,000 — 01-5
J. W. Patten and W. T. Pawlewicz

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 (Al, Cr, Ni) include: columnar growth impingement boundaries, defects vs. deposit integrity, diffusion, and deposited material near the substrate-deposit interface. Study areas for insulators (ZrO_2) include: stoichiometry, structure, properties, and adherence to metallic substrates. Sputtering parameters to be studied include: deposition rate, substrate temperature, bias, and oxygen partial pressure.

219. OPTICAL LASER MATERIAL STUDY — $120,000 — 02-2
J. S. Hartman and M. A. Lind

Evaluate stability of the metal/substrate interface in deposited mirrors subjected to environmental stresses (temperature, humidity, UV radiation) associated with extra terrestrial applications; determine bonding mechanisms for silver/substrate adhesion; preparation and evaluation of mirrors as a function of (1) substrate material (simple crystalline: quartz, amorphous: fused silica, and complex: soda-lime glass); (2) substrate preparation (abrasion, chemical cleaning, sputter etch); and (3) silver deposition techniques (wet chemistry, e-beam, rf sputtering); sample evaluation including ellipsometry, AES, SIMS, ESCA, optical properties (spectral reflectivity and scattering).

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

Optical property-materials property relationships for thin films and multilayer stacks; control of materials properties through understanding of reactive sputtering process; oxides of Ti, Zr, Hf, Ta, Nb, Si, Al, In, Sn, Y, La, and Mg; complex refractive index, spectral dependence of absorption edge, scattering, optical homogeneity and uniformity; structure, microstructure, stoichiometry, composition, purity, surface topography; transmission/reflection spectrophotometry, x-ray diffraction, TEM, SEM, XRF, Nomarski microscopy.

PACIFIC NORTHWEST LABORATORY (continued)

221. NANOMETER MACHINING AND GRINDING DEVELOPMENT $280,000 02-5
D. M. Miller and N. Laegreid

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 limitions. Development of grinding capability for hard and brittle materials.

SANDIA LABORATORIES
P. O. Box 5800
Albuquerque, New Mexico 87115

John Galt - Phone (FTS) 475-4669 or (505) 264-4669

222. STRESS CORROSION CRACKING AND ELECTROCHEMISTRY OF TRANSIENT CORROSION PROCESSES — $180,000 — 01-2
W. H. Smyrl

Crack propagation behavior of austenitic and ferritic stainless steels in molten salt environments; low melting $AlCl_3$-NaCl mixtures of known thermodynamic activity of Cl^-. Velocity of cracking varies weakly with Cl^- activity, but has strong dependence on electrochemical potential. Anodic dissolution mechanism for crack extension is being investigated. Influence of displacement reactions of the stainless steel with molten salt solvent is important at the corrosion potential, and is being studied experimentally with the Digital Faradaic Impedance technique. Modeling of the displacement reactions will be pursued. Digital Faradaic Impedance measurements on copper corrosion systems will be completed.

223. ION IMPLANTATION AND DEFECTS IN MATERIALS — $450,000 — 01-3
P. S. Peercy, S. M. Myers, H. J. Stein, S. T. Picraux, K. L. Brower, C. B. Norris, D. M. Follstaedt, J. A. Knapp

Modification and analysis of near surface regions of solids are being studied using ion beam techniques. Implantation metallurgy: studies of unique metallurgical systems formed by ion implantation, formation of equilibrium and nonequilibrium alloys, and electron beam and laser annealing of ion implanted metals, measurement of diffusion coefficients, solubility, enthalpy and entropy of reaction, phase diagram determinations, investigations of solute trapping by TEM and diffraction, trapping of hydrogen and temper embrittling species in Fe alloys, and amorphous surface layers on Fe. Laser annealing of implanted and amorphous semiconductors is studied by H concentration measurements and bonding studies in crystalline and amorphous Si, and EPR and optical investigation of defects in laser annealed semiconductors.

224. EROSION AND WEAR IN A FLUID ENVIRONMENT — $150,000 — 01-5
R. E. Cuthrell, D. M. Mattox, E. Randich

Basic studies on the fracture, erosion and wear of surfaces in varying thermal and chemical environments. Effects of chemical environment on the fracture of brittle materials (chemomechanical effects) under well controlled environments using sensitive fracture detection techniques such as acoustic emission, exoelectron/exoion emission and photon emission. Substrate-coating interaction in the formation of adherent coating-substrate couples. Failure analysis of eroded surfaces and failed coating-substrate interfaces with modeling of the failure mechanisms.

SANDIA LABORATORIES (continued)

225. SEMICONDUCTORS FOR USE AT HIGH TEMPERATURES — $110,000 — 01-5
R. J. Chaffin, G. C. Osbourn, C. E. Barnes, I. J. Fritz, L. R. Dawson

Experimental and theoretical studies of bulk and interfacial high temperature properties of wide bandgap semiconductors such as GaP, GaAs and GaAlAs. Objective is identification of candidate materials and contact metallizations suitable for high temperature (to 500°C) active semiconductor devices. Studies include transport, optical and defect (both thermal and athermal) properties. Emphasis is on defects in device-like structures, such as defects generated at interfaces between dissimilar materials and as influenced by mechanical stresses and electrical current (athermal) effects.

226. SURFACE PHYSICS RESEARCH — $180,000 — 02-2
M. L. Knotek, D. R. Jennison, J. E. Houston, R. R. Rye, J. A. Panitz, G. L. Kellogg

Studies are being conducted of the interaction of molecules and biomolecules with metal surfaces using the imaging and mass spectrometric capabilities of the Field-Ion/Field-Desorption Microscope. Experimental and theoretical procedures are also being developed for retrieving information on the local chemical environment of adsorbed atoms on solid surfaces using electron spectroscopic techniques. Utilizing gas phase molecular species as "absolute" standards, Auger Electron Spectroscopy and theoretical analysis are being used to characterize the local chemical environment of adsorbed species. The newly developed Pulsed Laser Atom Probe is being applied to the study of adsorption and reaction intermediates of molecular adsorbates on well defined transition metal surfaces.

227. DEVELOPMENT OF A FIELD-DESORPTION MICROSCOPE FOR SURFACE IMAGING — $170,000 — 02-5
J. A. Panitz

An instrument is being developed which utilizes field-desorption techniques to obtain images on the morphological structures of surfaces and biomolecular adsorbates. The apparatus will include the capability of time-of-flight mass analysis of desorbed species, sample surface dosing of biomolecular species without breaking vacuum and the ability to digitally store and manipulate two-dimensional image data.

SANDIA LABORATORIES (continued)

228. HYDROGEN PRODUCTION BY SOLAR PHOTO-ASSISTED ELECTROLYTIC DECOMPOSITION OF WATER — $145,000 — 02-2

M. A. Butler, D. M. Haaland, D. S. Ginley, G. W. Arnold

The basic mechanisms of photocatalytic and photosynthetic reactions at semiconductor/electrolyte interfaces are being investigated with emphasis on the charge transfer process. The roles of ion injection and exchange at the interface are being explored as mechanisms for modifying electrode properties. Photoresponse (both above and below the band gap), electrochemical techniques, fourier transform infrared and ion scattering techniques are used to delineate the interfacial effects. Ion implantation is being used to produce both chemically modified and structurally modified (amorphous) surface layers.

229. STUDIES OF THE VAPOR PHASE OF THE CHEMICAL-VAPOR-DEPOSITION PROCESS — $135,000 — 02-5

P. J. Hargis, A. W. Johnson, M. J. Kushner, M. E. Coltrin

Studies of important vapor-phase reactions and the condensation process during CVD processing of thin-film photovoltaic cells; measurements of major and trace species densities, gas temperature and fluid dynamic properties of the flow using Raman scattering, laser-induced fluorescence, and stimulated two-photon spectroscopy. Efforts to develop a predictive model and improved CVD processing techniques.

230. ELECTRON AND PHOTON-STIMULATED DESORPTION — $ 70,000 — 02-2

M. L. Knotek, G. M. Loubriel

Studies of the adsorption and reaction of H_2O, H_2, O_2, and other adsorbates with metal, metal oxide, and semiconductor surfaces are being carried out using the Electron- and Photon-stimulated desorption techniques (ESD and PSD). These investigations exploit the recent discovery that desorption occurs by Auger decay of radiation induced core-holes. Current experiments allow the extraction of site specific, adsorbate specific electronic and structural information relevant to the outermost layer. These techniques are uniquely sensitive to hydrogen and will be exploited in the study of hydrogen and its role in catalysis, corrosion, and semiconductor technology. PSD studies will utilize the Stanford Synchrotron Radiation Laboratory.

SANDIA LABORATORIES
Livermore, California 94550

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231. GASES IN METALS $200,000 01-2
W. D. Wilson G. J. Thomas
W. A. Swansiger M. I. Baskes
S. H. Goods

A joint theoretical and experimental program to increase fundamental understanding of the behavior of helium and hydrogen in metals and their influence on the mechanical properties of metals. Measurements and calculations of diffusion, trapping and clustering of helium in metals and alloys. Hydrogen phenomena are being examined utilizing transport measurements, autoradiography, electron microscopy and mechanical tests. Quantum theoretical calculations are performed in direct support of the experimental program.

232. DIAGNOSTICS FOR COMBUSTION MATERIALS RESEARCH $ 20,000 02-05
P. L. Mattern R. L. Farrow
R. E. Benner J. C. F. Wang

A program to develop and evaluate advanced, primarily in-situ diagnostics techniques for combustion-related materials research. Limitations and capabilities will be assessed in relation to a DBES-supported program to study materials in hot, corrosive/erosive environments. Raman backscattering spectroscopy will be evaluated as a remote probe of surface oxide behavior. In addition to surface diagnostics, new methods for gas and particulate temperatures, densities, and species will be developed and implemented where necessary. Fully developed methods will be installed at the Materials Research Combustion Simulator Laboratory at the Combustion Research Facility.

233. PROTECTIVE BARRIERS AND COATINGS FOR COMBUSTION MATERIALS $ 30,000 01-1
P. L. Mattern R. W. Mar
R. E. Benner R. L. Farrow
A. S. Nagelberg

A long-term, materials-oriented program to study corrosive/erosive processes at high temperatures. The Materials Research Combustion Simulator, a facility for simulating relevant combustion environments, will be developed and installed at the Combustion Research Facility at Sandia National Laboratories in Livermore. Initial emphasis will be given to the study of hot corrosion and gas phase oxidation in materials and coatings for use in coal-fired turbines. Advanced optical diagnostic methods will be used to characterize the simulated environments, and to monitor surface processes during exposure.

SOLAR ENERGY RESEARCH INSTITUTE
Golden, Colorado 80401

B. L. Butler - Phone: (FTS) 327-1104 or (303) 231-1104

234. ADVANCED SOLAR ENERGY MATERIALS RESEARCH ON THE DEGRADATION OF MIRROR AND POLYMERIC MATERIALS — $250,000 — 01-1
A. W. Czanderna

Mechanisms of materials degradation affecting the performance in solar energy conversion systems; interface studies in the glass/silver and silver/copper systems; polycrystalline silver films characterized for reflectance, topography, structure, composition and adhesion; corrosion reactions in aqueous solutions studied by both ac and dc electrochemical monitoring, weight changes, film thickness and in situ optical measurements in chemical cells; gas shape reactions of silver with atmospheric gases in flow environments in a surface analysis system; stability of polymer/silver interfaces.

SECTION B

Contract Research
(Primarily Universities)

This information was prepared by the technical monitors from material available in the contract documents. There is considerable 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 SURFACES AND DEFECTS IN CRYSTALS — $ 70,995 — 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.

UNIVERSITY OF ARIZONA — $139,823 — 02-2

302. CHEMICAL VAPOR DEPOSITION OF AMORPHOUS SILICON FOR PHOTO-THERMAL SOLAR ENERGY CONVERTERS
Bernhard O. Seraphin - Optical Sciences Center
Phone: (602)-626-2263

Production by chemical vapor deposition (CVD) of thin film amorphous silicon (a-Si) suitable for use as the solar absorber layer in photo-thermal converter stacks operating at temperatures above 550^{o}C. This is to be accomplished by controlling the conditions of CVD and by alloying the a-Si with elements such as C, N, O, B and/or Ge which may either retard crystallization of the a-Si or enhance solar absorptance or both. Characterization of the films is made by X-ray crystallography, high temperature spectrophotometry, SEM, direct chemical analysis, nuclear reaction depth profiling, and others.

BOSTON UNIVERSITY — $ 42,420 — 02-3

303. INFRARED ABSORPTION SPECTRUM OF FREE CARRIERS IN POLAR SEMICONDUCTORS
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 fields or high power lasers.

BROWN UNIVERSITY

304. A COMBINED MACROSCOPIC AND MICROSCOPIC APPROACH TO THE FRACTURE OF METALS — $152,600 — 01-2

R. J. Asaro - Division of Engineering
Phone: (401)-863-2317
J. Gurland - Division of Engineering
Phone: (401)-863-2628
J. R. Rice - Division of Engineering
Phone: (401)-863-2866

Analysis of deformation and fracture mechanisms in ductile alloys, principally steels; correlation of microstructure with crack initiation, crack growth, and fracture toughness; contributions of grain boundary diffusive flow and power law creep to void formation and linkage in creep rupture; environment-accelerated failure and interfacial decohesion, with emphasis on H_2 effects; numerical analysis of stable crack growth.

CALIFORNIA INSTITUTE OF TECHNOLOGY

305. STUDIES OF ALLOY STRUCTURE AND PROPERTIES — $195,000 — 01-1

William L. Johnson - Division of Engineering and Applied Science
Phone: (213)-975-6841 X1433

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 Mossbauer 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 Mossbauer spectroscopy, internal friction and positron annihilation spectroscopy.

306. THE PRESSURE DEPENDENCE OF THE MECHANICAL PROPERTIES OF POLYMERS — $ 54,970 — 01-2

N. W. Tschoegl - Dept. of Chemistry and Chemical Engineering
Phone: (213)-795-6811 X1676

Development of constitutive equations describing time-temperature-pressure effects on creep relaxation in elastomers; 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 $ 72,000 (14 months) 01-3

307. AN INVESTIGATION OF THE ROLE OF SINTERING IN GAS-SOLID INTERACTIONS
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. Influence of surface transport and bulk transport sintering on the kinetics of dissociation reactions of the type $CaCO_3(s) \rightleftharpoons CaO(s) + CO_2(g)$, and of reduction reactions of the type $FeO(s) + H_2(g) \rightleftharpoons Fe(s) + H_2O(g)$. Morphological changes (surface area, pore size, and overall porosity) will be measured and related to changes in the rates and reversibility of interactions of the types indicated above.

308. RADIATION DAMAGE AND ENVIRONMENTAL EFFECTS IN HIGH LEVEL WASTE STORAGE GLASSES USING TRANSMISSION ELECTRON MICROSCOPY $ 63,188 01-1
D. G. Howitt - Dept. of Mechanical Engineering
Phone: (916)-752-0580

Comparative evaluation of the response of H. L. W. S. G. (high level waste storage glasses) and candidate crystalline materials 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 including phase separation, precipitation, devitrification, particle size, and composite annealing temperatures on the properties of H.L.W.S.G. Experimental efforts will involve transmission, high voltage, and analytical electron microscopy, alpha, neutron, electron, and heavy ion irradiation, and leaching experiments.

309. DEFORMATION MECHANISMS AND FAILURE MODES IN SUPERPLASTICITY $ 57,000 01-2
A. K. Mukherjee - Dept. of Mechanical Engineering
Phone: 916)-752-0580

Experimental and analytical study of superplastic deformation of metals; determination of superplasticity flow parameters for Al-Zn alloys; influence of prior thermomechanical processing and competing flow mechanisms, e.g., cross-slip, on superplastic forming.

UNIVERSITY OF CALIFORNIA/IRVINE $ 62,778 02-2

310. INTERACTION OF LOW ENERGY ELECTRONS WITH SURFACE LATTICE VIBRATIONS
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 $ 88,586 01-4

311. IRRADIATION-INDUCED PRECIPITATION IN PALLADIUM-BASE ALLOYS
A. J. Ardell - Materials Dept.
Phone: (213)-825-2942

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; TEM, analytical electron microscopy and HVEM.

UNIVERSITY OF CALIFORNIA/SAN DIEGO $175,000 02-2

312. THE RESPONSE OF SUPERCONDUCTING TO VARIATIONS IN IMPURITY CONTENT AND APPLIED PRESSURE
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.

313. RESEARCH ON THE THERMOPHYSICAL PROPERTIES OF MATERIALS — $289,079 — 02-5

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

Studies of the principles of liquids working in heat engines will be continued and extended as follows: 1) Thermodynamic and kinetic properties of electrically insulating fluids will be obtained in the general vicinity of the critical point with emphasis on the region $T < T_c$ and pressures up to several times P_c; 2) These liquids will be assessed from a perspective of heat and work for application in heat engines operating on the Malone principle. The temperature range for this work will generally span a range of $\pm 50^{o}C$ around ambient temperature; 3) Liquid metals will be studied for use in a Malone-type engine having the remote end up to $600^{o}C$ above ambient temperature, thereby elucidating some of the essential qualities of engines using liquids; 4) Means will be explored by which heat engines using liquids can be operated without using gears or a flywheel; 5) Schemes will be sought for eliminating built-in imperfections in the Malone-concept thermodynamic pile. Additional studies of heat transfer will include an investigation of the onset of convective and other instabilities in a model system consisting of a dilute solution of ^{3}He in ^{4}He.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA — $ 67,181 — 02-2

314. RESONANCE STUDIES OF SUPERIONIC CONDUCTORS

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

NMR and EPR study of superionic and related compounds; EPR of ion interchange in rutile structure crystals. Study of the transverse and longitudinal relaxation rates of F^{19} in Mn doped PbF_2 as a function of temperature and NMR resonant frequency; use of the frequency dependence of EPR to study the spectral density function in Pb_2MnF_6; ionic conductivity of Bi doped PbF_2; computer simulation of the NMR and EPR spectra.

CARNEGIE INSTITUTE OF WASHINGTON — $ 94,446 — 02-2

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

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

Investigation of the properties of solid hydrogen in the pressure range 1 bar to 1.2 M bar. The Raman spectrum will be measured between 55 Kbar and 1.2M bar to provide data on H-H bond breaking. Comparative density measurements, at pressure, will be attempted. Specific volumes at pressure will be deduced from X-ray diffraction measurements and Brillouin scattering data, at pressure, will be taken to determine phase transition initiations and possible changes to the metallic state.

CARNEGIE-MELLON UNIVERSITY $ 53,648 (15 months) 01-1

316. KINETICS, MORPHOLOGY AND THERMODYNAMICS OF SOLID-LIQUID TRANSITION OF NON-METALS
R. G. Sekerka - Dept. of Metallurgy and Materials Science
Phone: (412)-578-2700

Kinetics, morphology, and thermodynamics of the solid-liquid transition in non-metals with emphasis on solid-liquid interface phenomena. Measurement of solid-liquid surface tension by the grain boundary groove technique and theoretical analysis of that technique for anisotropic materials. Modeling of the thermodynamics of solids and solid surfaces, and application to the solidification of ceramics.

317. FUNDAMENTAL STUDIES OF EROSION AND EROSION/CORROSION FOR COAL GASIFICATION SYSTEMS $ 55,000 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

Modeling particulate erosion of metals in terms of deformation and low cycle fatigue characteristics; 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, Cu-Al alloys, steels; techniques - laser interferometry, electron microscopy, finite element analysis.

CASE WESTERN RESERVE UNIVERSITY $ 81,000 01-3

318. STUDY OF COUPLED DIFFUSION PHENOMENA IN MULTICOMPONENT GLASSES AND GLASS FORMING LIQUIDS
A. R. Cooper - Dept. of Metallurgical and Materials Sciences
Phone: (216)-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 the 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.

319. ENVIRONMENTAL REACTIONS AND THEIR EFFECTS ON MECHANICAL BEHAVIOR OF METALLIC MATERIALS — $ 64,500 — 01-2

R. Gibala - Dept. of Metallurgy and Materials Science
Phone: (216)-368-4210

In-situ HVEM study of H_2 effects on deformation and fracture of steels; primary and secondary crack paths in high strength martensitic steels; experimental investigation of low temperature tensile ductility in Nb; effect of strain fields near internal precipitates (e.g., hydrides), surface coatings, and ion-implanted layers on alloy flow stress.

320. PLASTIC DEFORMATION IN OXIDE CERAMICS — $ 76,500 — 01-2

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

High temperature plastic deformation in oxygen-rich UO_{2+x}, and the formation of CS planes in TiO_{2+x}. Transmission electron microscopy of UO_{2+x} to study dislocation substructures produced during deformation and of TiO_{2+x} to study the mechanism controlling the formation of CS planes. Kinetics of annihilation of dislocation debris in UO_{2+x} as a function of stoichiometry. Microstructural evolution in MgO-$MgAl_2O_4$ fusion-cast refractories, specifically the precipitation of MgO from MgO-rich Mg-Al spinel solid solutions.

321. EXPERIMENTS IN HIGH VOLTAGE AND ANALYTICAL ELECTRON MICROSCOPY — $117,000 — 01-4

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

Effects of electron irradiation on the structure of ceramics using high voltage electron microscopy (HVEM) as well as experiments using neutron irradiation. HVEM experiments include (1) threshold displacement energy determination as a function of orientation, impurity content, and temperature, (2) quantitative studies of defect clustering and radiation-enhanced precipitate growth in various alloys, and (3) irradiation effects in ceramics. Displacement and ionization damage in ceramics, including (1) metamictization in SiO_2, B_2O_3, BeF_2, and various silicates, and (2) analysis of defect aggregation. Dislocation loop growth kinetics to determine defect migration energies in simple oxides such as MgO and Al_2O_3. Radiation-induced phase decomposition in double oxides such as $MgAl_2O_4$ and Mg_2SiO_4. Vacancy condensation leading to void formation in oxides such as Al_2O_3 and BeO which are particularly susceptible to radiation swelling. Nature of defect stabilization in more complex ceramic systems such as Y_2O_3, $Y_2Al_5O_{12}$, and Si_3N_4 which are notably resistant to swelling.

CATHOLIC UNIVERSITY OF AMERICA

322. IONIC TRANSPORT AND ELECTRICAL RELAXATION IN GLASS — $ 69,000 (16 months) — 01-3
C. T. Moynihan - Vitreous State Laboratory
Phone: (202)-635-5328

Ionic transport and electrical relaxation in glass; molecular dynamics computer simulation; dielectric relaxation as a function of alkali content; mixed alkali effect.

UNIVERSITY OF CINCINNATI

323. FLUX PINNING AND FLUX FLOW STUDIES IN SUPERCONDUCTORS USING FLUX FLOW NOISE TECHNIQUES — $ 62,234 — 02-2
W. C. H. Joiner - Dept. of Physics
Phone: (513)-475-2232

The objective of this work is to study flux pinning and the dynamics of flux flow in type II superconductors. Superconducting alloy samples of $Pb_{1-x}In_x$ are prepared containing various metallurgical defects and exhibiting different critical current characteristics resulting from the defect structure and the flux flow noise power spectrum is studied. This gives information on flux bundle size, transit time, pinning forces and other flux flow parameters. Magnetic field dependence of flux pinning sites, pinning force curve, surface pinning effects, surface grooving effect are examples of particular phenomena to be studied.

COLORADO ENERGY RESEARCH INSTITUTE

324. HYDROGEN AND METHANE SYNTHESES THROUGH RADIATION CATALYSIS — $ 73,643 — 02-2
J. DuBow, Dept. of Electrical Engineering, Colorado State University
Phone: (303)-491-8235

Ionizing radiation has been shown to increase reaction rates by up to two orders of magnitude. The radiation generates electron-hole pairs through optical or radioactive stimulus and subsequent excitation via sub-damage threshold radiation enables the continuous generation of metastable high energy carrier pairs. This research is involved with a study of radiation-induced catalysis examining mechanisms of energy transfer from the catalyst to its adsorbed reactant in an ionizing radiation environment. Among the oxide catalysts employed are V_2O_5(E_g = 2.3eV), TiO_2 (3.0 eV), SnO_2 (4.3 eV), and HfO_2 (5.6 eV). An attempt will be made to modify the catalysts by appropriate doping, e.g., Al_2O_3 and Ga_2O_3 will be used as dopants in ZnO. The physical form of the catalysts will also be varied.

COLORADO SCHOOL OF MINES

325. FERROUS ALLOY METALLURGY - LIQUID LITHIUM CORROSION AND WELDING — $119,681 — 01-5

D. L. Olson - Dept. of Metallurgical Engineering
Phone: (303)-279-0300, X787
D. K. Matlock - Dept. of Metallurgical Engineering
Phone: (303)-279-0300, X775

Mechanical behavior of ferrous alloys in liquid lithium environments and welding of dissimilar metal joints; facility to test reactive metals such as lithium; fatigue crack growth in 304 and 2 1/4 Cr - 1 Mo steels in liquid Li; microstructure and mechanical properties of dissimilar weldments of 2 1/4 Cr - 1 Mo to 316 stainless steel; thermodynamic modeling to predict microstructure of weldments.

UNIVERSITY OF COLORADO

326. CRITICAL SCATTERING OF LASER LIGHT BY FLUID FILMS AND INTERFACES — $200,655 (2 years) — 02-2

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

Applications of laser intensity-autocorrelation spectroscopy to study the dynamical behavior of fluid films. Measurements of the intensity-autocorrelation function of light scattered by critical fluid films for address of the question, what are the effects of restricted geometry on the dynamical properties of a critical fluid system? Investigation of the autocorrelation function of light from films formed of monodisperse colloidal suspensions of charged microspheres over a particle density regime spanning gas-like, liquid-like, and crystalline phases. Study of the autocorrelation of light scattered from various fluid surface and model membranes. Ellipsometric studies of solid/critical fluid interfaces. Coexistence curve measurements on films of an upper critical curve binary fluid mixture to assess the generality of the previously observed finite size effects in films of the lower critical point system 2, 6-lutidine + water.

COLUMBIA UNIVERSITY

327. DEFECT INTERACTIONS AT HIGH CONCENTRATIONS IN SOLID-OXIDE ELECTROLYTES — $ 50,000 — 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 Ca; 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; defect structure in Bi_2O_3-based solid solutions, with the fluorite structures, having high conductivity. Electrode phenomena. Complex impedance plots and the "grain-boundary effect." Dielectric relaxation. Anelastic relaxation. Neutron scattering.

UNIVERSITY OF CONNECTICUT

328. ELECTRODE POLARIZATION STUDIES IN HOT CORROSION SYSTEMS — $ 56,600 — 01-3
O. F. Devereux - Dept. of Metallurgy
Phone: (203)-486-4714

Investigation of molten salt corrosion of Fe and Ni; electrode polarization measurements in carbonates having various H:O:S activities; determination of electrode reactions and their kinetics and energetics; sulfidation of Fe in gaseous environments.

329. ELECTRON-DISLOCATION INTERACTIONS AT LOW TEMPERATURES — $ 60,000 — 01-2
J. M. Galligan - Dept. of Metallurgy
Phone: (203)-486-3541/4623

Role of electron drag on dislocation mobility in metals. The superconducting-normal transition is exploited to alter the electronic state of a metal or alloy without changing the composition or microstructure, and plastic deformation is studied both above and below this transition. The contributions of electrons and phonons to mobile dislocation drag are thus separated and measured. The effects of applied magnetic fields on the electron drag on dislocations in metals in the normal state is also under investigation.

CORNELL UNIVERSITY

330. INFLUENCE OF GRAIN BOUNDARIES ON THE ELECTRICAL TRANSPORT PROPERTIES OF POLYCRYSTALLINE SI FILMS — $ 59,000 — 01-1
D. G. Ast - Dept. of Materials Science and Engineering
Phone: (607)-256-4140

Characterization of the structure and electrical activity of grain boundaries in hot-pressed Si; modification of boundary structure due to interactions with lattice dislocations; techniques used: TEM, electron beam induced charge in SEM.

331. INITIAL STAGES OF OXIDATION OF METALS — $ 105,600 — 01-1

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

Experimental study of oxide structure and growth kinetics, and changes therein with scale thickness, on Fe-Ni and Be crystals; techniques used: LEED, AES, TEM.

332. INELASTIC DEFORMATION OF NONMETALLIC CRYSTALLINE SOLIDS — $ 47,000 — 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 TiB_2 precipitates on such materials. Densification mechanisms and kinetics. Creep and constant compressive strain rate experiments. TEM-STEM analysis.

333. ENVIRONMENT AND FRACTURE — $ 81,500 — 01-2

H. H. Johnson - Dept. of Materials Sciences and Engineering
Phone: (607)-256-2323

Experimental investigation of H_2 permeation through metals, primarily steels; trapping sites, densities, and characteristic binding energies for dislocations and substitutional solute atoms; effect of prior cold work and applied stress level on H_2 trapping, solubility, and diffusivity.

334. MECHANICAL PROPERTIES OF CRYSTALLINE SOLIDS — $120,000 — 01-2

Che-Yu Li - Dept. of Materials Science and Engineering
Phone: (607)-256-4349
E. W. Hart - Dept. of Materials Science and Engineering and Theoretical and Applied Mechanics
Phone: (607)-256-4853
S. Mukherjee - Dept. of Theoretical and Applied Mechanics
Phone: (607)-256-7143

Development of a state variable description of non-elastic deformation in crystalline solids, modelling and experiments; constitutive equations for mechanical design applications; transient grain matrix deformation, Al, Ni and type 316 stainless steel; grain boundary sliding, Ni; grain boundary cavitation, zircaloys; numerical stress analysis methods; solution to inelastic boundary value problems using constitutive equations and stress analysis codes.

335. PROBABILISTIC MODELS OF THE STRESS-RUPTURE OF COMPOSITE MATERIALS — $ 67,300 — 01-2
S. L. Phoenix - Sibley School of Mechanical & Aerospace Engineering
Phone: (607)-256-3462

Analysis of tensile and stress-rupture strengths of fiber reinforced polymer composites using probabilistic modelling based on fiber strength distribution; local vs equal load sharing rules; failure criteria as a function of composite size; asymptotic solutions.

336. HIGH TEMPERATURE MECHANICAL BEHAVIOR OF SILICON NITRIDE — $ 87,465 — 01-2
R. Raj - Dept. of Materials Science and Engineering
Phone: (607)-256-4040

Mechanical behavior of ceramics which contain a residual glass phase in the grain boundaries. Kinetics of dissolution/precipitation (ceramics $\leftrightarrows$ glass), glass viscosity, and grain boundary sliding. Mechanical behavior under confining pressure. Thermal shock behavior of glass ceramics. Principal materials under investigation are hot pressed Si_3N_4 and β-spodumene lithia-aluminosilicate glass.

337. DEFECTS IN METAL CRYSTALS — $215,000 — 01-4
David N. Seidman - Dept. of Materials Science and Engineering
Phone: (607)-256-2365

Properties of crystal defects in metals and semiconductors; properties of light gases (He, H and Ne) in metals; low temperature adsorption of H on W surfaces; non-equilibrium segregation of solute atoms to voids during irradiation; radiation damage; experimental techniques include field-ion microscopy, atom-probe field-ion microscopy, transmission electron microscopy and electrical resistivity; AP/FIM imaging of semiconducting materials - silicon, gallium phosphide and gallium arsenide.

DARTMOUTH COLLEGE

338. THEORY OF ELECTRON-PHONON SCATTERING EFFECTS IN METALS — $ 23,894 — 02-3
W. E. Lawrence - Dept. of Physics and Astronomy
Phone: (603)-646-2963

It is proposed to continue studies of the quasi-particle scattering times of the noble and polyvalent metals. The transport problem will be studied by means of the diffusion model. Electron-electron scattering will be studied further in the noble metals, with regard to deviations from Matthiessen's rule when electron-phonon scattering is present. Non equilibrium studies in general will be continued and new studies begun for superconductors. In the latter case variational methods will be used.

339. SUPERCONDUCTIVITY IN FILAMENTARY EUTECTIC COMPOSITES — $ 38,165 — 02-2

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

This program involves an experimental and theoretical study of the electrical and thermal conductivity very close to the superconducting transition temperature in eutectics such as Nb-Th which consist of tiny Nb (10 to 100 nm diameter) filaments in a matrix of Th. The purpose of the study is to understand the role of thermodynamic fluctuations in the behavior of these materials, which are expected to behave in many respects as one dimensional superconductors. The magnetic susceptibility shows essentially perfect diamagnetism below 7K. This is in contradiction to theories of the proximity effect which predict a sharp decrease in the transition temperature for samples with a radius smaller than the coherence length. This may be an indication of a new mechanism for coupling filaments not described by the Josephson effect.

UNIVERSITY OF DELAWARE

340. ANALYSES OF FAILURE MODES IN SHORT FIBER REINFORCED THERMOPLASTICS — $ 30,000 — 01-2

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

Statistical modelling of fiber distribution, the strain field around fiber ends, and crack initiation and extension in a matrix exhibiting elastic-plastic behavior.

341. RADIATION EFFECTS IN AMORHPOUS METALLIC ALLOYS — $ 66,322 — 02-2

Richard B. Murray - Dept. of Physics
Phone: (302)-738-2147
David G. Onn - Dept. of Physics
Phone: (302)-738-2680
John J. Kramer - Dept. of Electrical Engineering
Phone: (302)-738-8170

The principal investigators propose to observe the effects of irradiation of amorphous alloys of the composition $Fe_xNi_{80-x}P_{14}B_6$ with high and low energy protons as well as low energy electrons, and to identify the structural changes that are responsible for the observed effects. The effects measured will be electrical resistivity, Curie temperature, saturation magnetic moment, magnetic domain structure, and crystallization behavior.

DREXEL UNIVERSITY

342. STRAIN HARDENING AND DUCTILITY OF IRON: AXISYMMETRIC VS. PLANE STRAIN ELONGATION — $ 53,000 — 01-5

G. Langford - Dept. of Materials Engineering
Phone: (215)-895-2330

Stress-strain-structure determination of Fe and steels after axisymmetric, plane strain, and shear deformations; modelling complex forming operations in terms of simpler ones; homogeneous slip vs shear band formation; technique used: HVEM.

EMORY UNIVERSITY

343. FAR INFRARED STUDIES OF SUPER-CONDUCTING V_3Si, Nb_3Ge and Nb — $ 45,878 — 02-2

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

Measurements of optical absorption in the far infrared are to be made on four superconductors, V_3Si, Nb_3Ge, Nb and granular NbN as a function of temperature near the superconducting transition temperature. The data will be used to elucidate the connection between the transition temperature and various features of the phonon and electron density of states functions. Also included is the development of new methods of making FIR measurements.

FLORIDA STATE UNIVERSITY

344. POLYMERS IN MECHANO-CHEMICAL SYSTEMS: STRUCTURE-PROPERTY REQUIREMENTS — $ 59,000 — 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 stress; a description of the morphological forms that result, and their influence on mechanical properties. Optimization of the functioning of mechano-chemical systems of polymers.

UNIVERSITY OF FLORIDA

345. SYNTHESIS AND CHARACTERIZATION OF NOVEL POLYMERS FROM NON-PETROLEUM SOURCES — $ 95,000 — 03-3

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

Synthesis 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.

346. DEFORMATION PROCESSES IN REFRACTORY METALS — $ 32,100 — 01-2

R. E. Reed-Hill - Dept. of Materials Science and Engineering
Phone: (904)-392-1455

Dynamic strain aging and slow strain rate embrittlement in Nb-O from ambient to 700°C and in V-O aged under load in the Snoek ordering region; identification of fracture and dislocation pinning mechanisms as well as the effects of interstitial clustering and transport thereon; techniques used -- internal friction.

GENERAL ELECTRIC CORPORATE RESEARCH AND DEVELOPMENT

347. LOCAL ATOMIC AND ELECTRONIC STRUCTURE IN GLASSY METALLIC ALLOYS — $ 95,888 — 02-2

Eric Lifshin - Materials Characterization Laboratory
Phone: (518)-385-8556
R. P. Messmer - Materials Characterization Laboratory
Phone: (518)-385-8488
Joe Wong - Materials Characterization Laboratory
Phone: (518)-385-8463

This is a program combining experimental and theoretical techniques for studying the local electronic and atomic structure of glassy metal alloys. Specifically, the very recently exploited experimental methods known as EXAFS (extended x-ray absorption fine structure) will be used in conjunction with the Stanford Synchrotron Radiation Laboratory (SSRL) to study the local atomic distribution in glassy metallic alloys containing Fe, Ni, B, and P. (EXAFS studies will also be made on Ti-Cu, Zr-Fe, Zr-Co, Zr-Ni, Zr,Cu and Nb-Ni systems). The theory meanwhile will use the resulting atomic structure data as input to cluster calculations employing modern computationsl techniques from which electronic structure data such as density of states (DOS) and magnetic properties can be inferred.

348. A STUDY OF SOLID METAL/CERAMIC REACTIONS — $ 70,000 — 01-5

M. R. Jackson - Metallurgy Laboratory
Phone: (518)-385-8592
R. L. Mehan, Physical Chemistry Laboratory
Phone: (518)-385-8398

Characterization of the thermally-activated stress-assisted interaction of a model Ni-based Ni-Cr-Al alloy with hot-pressed SiC, hot-pressed Si_3N_4, and reaction bonded SiC, with particular consideration towards developing an understanding of the reaction kinetics, diffusive processes contributing to the reaction mechanism, and phase equilibria governing the sequence of reactions. Effects on reaction kinetics and mechanisms which result from a controlled alteration of phase equilibria achieved by modifying the surface chemistry of the aforesaid metallic and/or ceramic material. These surface chemistry modifications may consist of (a) relatively stable oxides such as Y_2O_3 and Al_2O_3 sputtered or plasma sprayed onto the above Si bearing ceramic substrates and (b) formation of refractory metal (such as Mo), silicide, carbide, or nitride layers on substrates of the above Ni-Cr-Al alloy.

GEORGIA INSTITUTE OF TECHNOLOGY

349. THE STRUCTURE AND REACTIVITY OF HETEROGENEOUS SURFACES AND STUDIES OF THE GEOMETRY OF SURFACE COMPLEXES — $104,000 — 02-3
U. Landman - Dept. of Physics
Phone: (404)-894-3368

An investigation of methods for the study of the geometry and dynamics of adsorbated on surfaces. Using a newly developed cluster migration technique and surface molecular dynamics such problems as diffusion, annealing and bimolecular surface reactions are being studied. Also a vibrational-phonon coupling model to explain thermal desorption is being developed. Impurity electronic states at semiconductor grain boundaries are being calculated.

350. INVESTIGATIONS OF INTERMETALLIC ALLOY HYDRIDING MECHANISMS — $ 82,000 — 01-1
B. R. Livesay - Applied Science Laboratory
Phone: (404)-894-3489

Mechanisms and kinetics of hydriding and dehydriding hydrogen storage alloys, viz., $La(Ni,Co)_5$, $SmCo_5$ and FeTi; apparatus includes an in-situ automatic torque magnetometer and microbalance, an in-situ four-point probe resistivity cell and in-situ thin film flexure measurement equipment; in-situ HVEM investigation so hydride platelets in $La(Ni,Co)_5$; post-hydriding TEM investigation, FeTi.

UNIVERSITY OF HOUSTON

351. MICROSTRUCTURAL STUDIES OF HYDROGEN AND OTHER INTERSTITIAL DEFECTS IN BCC REFRACTORY METALS — $ 70,000 — 02-2
Simon C. 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; interstitial-induced strain fields and changes in Fermi surface modification.

ILLINOIS INSTITUTE OF TECHNOLOGY

352. DIFFUSION MECHANISMS AND DEGRADATION OF ENVIRONMENTALLY SENSITIVE COMPOSITE MATERIALS — $ 53,000 — 01-2
L. J. Broutman - Dept. of Metallurgy and Materials Engineering
Phone: (312)-567-3049

Moisture diffusion and permeation in epoxies with various degrees of cross-linking and under a range of applied stresses; correlation of strength changes and dimensional instabilities in the epoxy with moisture-induced degradation of graphite fiber reinforced epoxy composites.

353. ELECTROCHEMISTRY OF ACETYLIDES, NITRIDES AND CARBON CATHODES IN MOLTEN HALIDES — $ 58,000 — 03-3

J. R. Selman - Dept. of Chemical Engineering
Phone: (312)-567-3037

EMF measurements on Ca-Al alloys in the temperature range 500-900°C, and diffusivity measurements of calcium in Ca-Al alloys. Synthesis and characterization of intercalation compounds of Ca and of Li with graphite, including kinetic studies of the processes by chronopotentiometry.

JOHNS HOPKINS UNIVERSITY

354. CONDENSATION PROCESSES IN COAL COMBUSTION PRODUCTS — $ 56,000 — 03-3

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

Studies of complex condensation processes occuring in coal combustion and gasification, with emphasis on non-equilibrium processes. Studies of thermal and electrical properties of aerosols, and on the kinetics of nucleation and chemical reactions in fly ash and silicates.

LEHIGH UNIVERSITY

355. ANALYTICAL STUDY OF DRAWING AND EXTRUSION OF SUPERCONDUCTING FILAMENTARY WIRE: FRACTURE PROBLEMS AND EVALUATION OF TEMPERATURE RISE — $ 81,000 — 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.

LEHIGH UNIVERSITY

356. PRESSURE SINTERING AND CREEP DEFORMATION - A JOINT MODELING APPROACH — $ 56,000 — 01-1

M. R. Notis - Dept. of Metallurgy and Materials Engineering
Phone: (215)-861-4225

Comparison of densification behavior during hot-pressing with deformation during creep; quantitative steoeology of the microstructure modification of doped oxide ceramics as a function of various densification parameters; quantitative studies of the microchemistry and fine structure of impurity doped hot-pressed specimens will be carried out by high resolution structural and chemical analysis techniques (STEM equipped with non-dispersive X-ray facilities) in order to examine grain boundary segregation phenomena and its relation to densification phenomena.

LOUISIANA STATE UNIVERSITY

357. INTER-SUBBAND OPTICAL ABSORPTION IN AN INVERSION LAYER ON A SEMICONDUCTOR SURFACE IN TILTED MAGNETIC FIELDS — $ 35,475 — 02-3

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

Inter-Subband Optical Absorption is observed when space charge accumulates at the interface between a semiconductor and an insulator and is important in MOSFET technology. Semiclassical theory cannot explain the observed optical absorption in this system. An attempt will be made to calculate the effect of a magnetic field on the exchange-correlation potential and other many body effects such as depolarization shifts and exciton-like shifts in order to resolve the discrepancy between theory and experiment. In addition, work will be done to determine the feasibility of obtaining useful information from Faraday rotation experiments in MOS systems.

UNIVERSITY OF MAINE

358. GROWTH AND CHARACTERIZATION OF TERNARY SEMICONDUCTOR COMPOUNDS PRODUCED BY MOLECULAR BEAM EPITAXY — $ 73,428 — 02-2

A. H. Clark - The Materials Science Institute
Phone: (207)-581-7745

Study the growth of selenium-based ternary semiconductors produced by molecular beam epitaxy (MBE); these semiconductors are of potential use in photovoltaic, electroluminescent and optomagnetic devices. The main questions addressed are the requirements and best methods for control of effusion rates, the nature of compounds formed due to deviations from stoichiometry, and the subsequent electrical, optical and magnetic properties of the epitaxial layers produced. Specific materials of current interest are $CuInSe_2$, $AgInSe_2$, $AgGaSe_2$, and the spinel $CdCr_2Se_4$.

UNIVERSITY OF MARYLAND

359. ADSORPTION OF METAL SURFACES — $129,725 — 02-2

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

Joint theoretical/experiment 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.

360. ALLOY STRENGTHENING DUE TO ATOMIC ORDER — $ 54,592 — 01-2

M. J. Marcinkowski - Dept. of Mechanical Engineering
Phone: (301)-454-2408

Modelling grain boundaries, interfaces, and cracks in metals in terms of dislocation arrays; use of energy minimization to establish crack stability under various conditions---monotonic vs reversed loading, tension vs shear stress states; development of scaling laws.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

361. MICROMECHANICAL MODELLING OF MICROSTRUCTURAL DAMAGE AT ELEVATED TEMPERATURE DURING CREEP OF SUPER-ALLOYS FOR ENERGY APPLICATIONS — $125,000 — 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 rupture of metals; strain concentrations at grain boundaries and triple points; influence of dispersed particles on boundary sliding and cavity formation; stress and strain fields around moving and stationary cracks subjected to load transients; confirmatory experiments, primarily with stainless steels, to measure cavitation kinetics, grain boundary sliding, and creep rates.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

362. KINETIC PROCESSES AT GRAIN BOUNDARIES — $134,801 — 01-1
R. W. Balluffi - Dept. of Materials Science and Engineering
Phone: (617)-253-3349

Kinetic processes such as diffusion and grain boundary motion at grain boundaries in metals and ceramics; experimental, analytical and computer simulation; intrinsic and extrinsic grain boundaries in MgO; grain boundary dislocations in plane matching grain boundaries; analysis and review of high angle grain boundaries as sources or sinks for point defects; simulation of the structure of vacancies in high angle grain boundaries.

363. PHYSICS AND CHEMISTRY OF PACKING FINE CERAMIC POWDERS — $ 80,000 (11 months) — 01-5
H. K. Bowen - Dept. of Materials Science and Engineering
Phone: (617)-253-6892

Application of synthesis aspects of colloid chemistry, mono-sized particulates, and paradigms for sintering to develop a scientific understanding for controlling green density. Determination of space charge or steric stabilization parameters for TiO_2 and Si_3N_4, measurement of colloidal ordering and controlled coagulation, and theoretical modelling of allowable particle size distribution for ordered structures.

364. PROCESSING STUDIES OF POWDER METALLURGICALLY PRODUCED HIGH TEMPERATURE ALLOYS — $ 48,000 — 01-2
N. J. Grant - Dept. of Materials Science and Engineering
Phone: (617)-253-5637

Powder metallurgical fabrication of Fe-, Ni-, and Co-base alloys; use of pulsed atomization process to modify composition and phase distribution from those of ingot stock; elevated temperature stress rupture behavior.

365. BASIC RESEARCH IN CRYSTALLINE AND NONCRYSTALLINE CERAMIC SYSTEMS — $545,000 — 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

High temperature electrical properties of MgO; mechanical properties of Al_2O_3; electrical properties of pure and doped UO_2; vacuum ultraviolet optical properties of Al_2O_3; calculations of defect structures in MgO; grain boundary and surface segregation in SiC; grain boundary grooving and surface diffusion in Al_2O_3; sintering of covalent materials; creep in MgO-doped Al_2O_3; deformation mechanism mapping for UO_2.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

366. INFLUENCE OF GASEOUS ENVIRONMENT ON NEAR THRESHOLD, LOW GROWTH RATE FATIGUE CRACK PROPAGATION — $ 67,900 — 01-2
R. O. Ritchie - Dept. of Mechanical Engineering
Phone: (617)-253-2311

Fatigue of both high strength martensitic steels and low strength ferritic steels studied in air and H_2 over a range of loads; effects of load ratio, ΔK, frequency, and H_2 permeation; relationship of corrosion fatigue to stress corrosion cracking; correlation with microstructural aspects such as prior austenite grain size, martensitic structure, and impurity segregation.

367. LOW TEMPERATURE AND NEUTRON PHYSICS STUDIES — $180,653 — 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.

368. SPECTROSCOPIC INVESTIGATIONS OF SMALL MOLECULE INTERACTIONS ON METAL OXIDE SURFACES — $ 75,000 — 03-1
E. I. Solomon - Dept. of Chemistry
Phone: (617)-253-4508
F. R. McFeely - Dept. of Chemistry
Phone: (617)-253-6106

Studies of the interaction of CO with a variety of low index ZnO surfaces, using both angular-resolved and angular-integrated UV photoemission. Derivation of alignment of CO with selected ZnO surfaces; poisoning of ZnO surfaces by adsorbed H_2O and NH_3.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

369. A BASIC STUDY OF HEAT FLOW IN FUSION WELDING — $ 84,800 — 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 electroslag and arc welding processes; heat and fluid flow for slag phase; heat loss with various weld geometries and base plate gaps; electrode melting rate and multiple electrode considerations; transient heat flows in arc welding; complementary experimental effort fabricating weldments in low alloy steels.

370. ELECTRONIC CONDUCTION IN SOLID OXIDE ELECTROLYTES — $ 70,000 — 03-3

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

Examination of ionic and electronic conductivity in ZrO_2, ThO_2, and HfO_2 at high temperatures and low oxygen partial pressures. Effect of doping by CeO_2 and its contribution to enhanced ionic conductivity. Measurement of A. C. conductance parameters related to electrical interface and grain boundary contributions to electrical properties.

371. HIGH TEMPERATURE PROPERTIES AND PROCESSES IN CERAMICS: THERMOMIGRATION — $ 70,000 — 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 Fe-Al spinels, KCl, UO_2, FeO, and NiO-CuO 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.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

372. FUNDAMENTAL INVESTIGATIONS OF THE OXIDATION OF ALLOYS IN MULTICOMPONENT GASEOUS ENVIRONMENTS — $ 75,000 — 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; Cr_2O_3 formation kinetics and structure, and transport of S through it; effect of preoxidation in pure O_2; techniques used--thermogravimetry, STEM, SAM.

UNIVERSITY OF MASSACHUSETTS

373. SYNTHESIS OF METASTABLE A-15 SUPERCONDUCTING COMPOUNDS BY ION IMPLANTATION — $ 37,170 — 02-2
M. T. Clapp - Dept. of Mechanical Engineering
Phone: (413)-545-2505

Synthesis of metastable A-15 superconducting compounds, in particular Nb_3, Si, Nb_3C, and Nb_3B. Technique involves starting with a stable high T_c substrate such as Nb_3Al, diffusion annealing to deplete the surface of Al, and then replacing the Al deficiency with Si, B, or C by sequential implantations at different doses and energies chosen to maintain the stoichiometry (25 atomic percent Al/Si, Al/C, or Al/B). Resulting disordered surface will be heat-treated to promote expitaxial recrystallization on the A-15 substrate. Characterization of resulting films: structure (reflection electron diffraction), composition (Auger and ion microprobe), and T_c.

MICHIGAN MOLECULAR INSTITUTE

374. RELATIONSHIPS BETWEEN PHYSICAL PROPERTIES OF POLYMERS AND CROSS-SECTIONAL AREA PER POLYMER CHAIN — $ 26,000 — 03-1
R. L. Miller, Sr.
Phone: (517)-631-9450
R. F. Boyer
Phone: (517)-631-9450

Compilation of data on property-structure relationships of macromolecular systems, with emphasis on correlations between physical properties and cross-sectional area per polymer chain. Experimental work is undertaken when gaps or discrepancies in data are found. Emphasis on the prediction of physical properties.

MICHIGAN TECHNOLOGICAL UNIVERSITY

375. A STUDY OF GRAIN BOUNDARY SEGREGATION USING THE AUGER ELECTRON EMISSION TECHNIQUE — $ 56,000 — 01-2

D. F. Stein - Dept. of Metallurgical Engineering
Phone: (906)-487-2440
L. A. Heldt - Dept. of Metallurgical Engineering
Phone: (906)-487-2630

Effect of grain boundary orientation and structure on the extent of segregation; environment assisted fracture under multiaxial loading; stress corrosion cracking, theory and experiment; Auger electron spectroscopy; segregation of S in Mo, Bi in Fe, S in Fe; stress corrosion cracking of aluminum bronzes; hydrogen embrittlement of copper alloys and pure iron; liquid and solid metal embrittlement as affected by grain boundary segregation; embrittlement of P bearing Ni-Cu alloys by H and by liquid Hg.

UNIVERSITY OF MICHIGAN

376. EFFECT OF CRYSTALLIZATION OF GRAIN BOUNDARY PHASE ON THE HIGH TEMPERATURE STRENGTH OF SILICON NITRIDE CERAMICS — $ 56,000 — 01-1

T. Y. Tien - 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 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 MINNESOTA

377. NEAR NEIGHBOR SEPARATIONS OF SURFACE ATOMS — $ 79,870 — 02-2

P. I. Cohen - Dept. of Electrical Engineering
Phone: (612)-373-3025

Experiments will be performed for a series of representative clean and monolayer covered single-crystal surfaces to demonstrate the feasibility of using the extended fine structure observed in electron scattering experiments to determine surface near neighbor spacings. Two approaches will be taken: (1) an ultrahigh-vacuum-compatible surface-barrier electron detector will be constructed to measure the extended fine structure that has been observed to investigate the extended fine structure in high energy electron scattering at glancing angles from surfaces.

UNIVERSITY OF MINNESOTA (continued)

378. A MICROSTRUCTURAL APPROACH TO FATIGUE CRACK PROCESSES IN POLYCRYSTALLINE BCC MATERIALS — $ 58,100 — 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; influence of mechanical properties--strain rate sensitivity, flow stress and its temperature dependence, monotonic vs cyclic loading, and ΔK; effects of microstructural features such as grain size and slip characteristics; modelling in terms of dislocation dynamics and fracture toughness parameters; techniques used: electron channeling, TEM, SEM.

379. FAR INFRARED AND THERMAL STUDIES ON LOW TEMPERATURE MATERIALS — $ 49,806 — 02-2

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

Design and fabrication of a modulated interference FIR spectrometer which will be used to measure the optical absorption coefficients directly for such materials as V_3Si, V_3Ge, Nb_3Ge, Nb_3Sn, chevrel phase compounds, rare earth rhodium borides, and superionic conductors. Furthermore, measurements of heat capacity and thermal and electrical transport coefficients of V_3Si will be made in order to quantify the behavior of the martinsitic phase transformation and second superconducting transition which occurs in this material. Careful attention must be payed to stoichiometry in this material.

380. CORROSION PROCESSES AND ENERGY SYSTEMS — $980,000 — 01-1

R. W. Staehle - Dept. of Chemical Engineering and Materials Science
Phone: (612)-373-2955
W. W. Gerberich - Dept. of Chemical Engineering and Materials Science
Phone: (612)-373-4829
R. Oriani - Dept. of Chemical Engineering and Materials Science
Phone: (612)-373-4864

Research and technology transfer in corrosion; surface spectroscopy of metals, polymers and metal-polymer interactions; corrosion resistance imparted to metal surfaces by plasma processed polymer films; ESCA and infrared spectroscopy; high temperature sulfidation and plasma spray coatings; corrosion behavior of Fe-Cr with Ni additions in dilute H_2S atmospheres; multilayer coatings of metals and ceramics; thermodynamic and cracking aspects of hydrogen in BCC metals; craze phenomena in glassy polymers; construction of a high temperature solar furnace.

UNIVERSITY OF MISSOURI

381. DEVELOPMENT AND CHARACTERIZATION OF HIGH TEMPERATURE ELECTRICALLY CONDUCTING OXIDES — $ 83,730 (11 months) — 01-3

H. E. Anderson - Dept. of Ceramic Engineering
Phone: (314)-341-4401
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 oxides Cr_2O_3, NiO, $LaCrO_3$, and $YCrO_3$. Experimental aspects include specimen preparation, thermogravimetric measurements, X-ray diffraction, transmission electron microscopy, and magnetic susceptibility, Hall, conductivity, and Seebeck measurements.

382. ELECTRONIC PROPERTIES OF AMORPHOUS SILICON DIOXIDE AND METALLIC IONS IN SILICATE GLASSES — $ 27,373 (16 months) — 01-1

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

The electronic properties of crystalline silicon dioxide, silicon nitride, amorphous silicon dioxide, and silicate glasses are to be studied by means of a first principles orthogonalized linear combination of atomic orbitals (OLCAO) method. Special emphasis will be placed on the nature and location of impurity states of various ions in the silicate glass network as well as the interaction between the impurity ions and their host.

NATIONAL BUREAU OF STANDARDS

383. STUDY OF ECONOMIC AND SAFETY COSTS OF FRACTURE — $ 50,000 — 01-2

J. B. Wachtman, Jr. - Center for Materials Science
Phone: (301)-921-2891

Two year study on the impact of fracture on the U.S. economy; study to include total cost, present reducible cost and future reducible cost, i.e., measure the potential benefit of technology transfer programs in fracture technology; several agencies involved in the study.

NEW MEXICO INSTITUTE OF MINING AND TECHNOLOGY

384. MICROSTRUCTURAL AND MECHANICAL PROPERTY STUDY OF SOLAR ENERGY COLLECTORS — $ 81,180 — 01-1
O. T. Inal - Dept. of Metallurgical and Materials Engineering
Phone: (505)-835-5229

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.

385. CHARACTERIZATION OF EXTRINSIC GRAIN BOUNDARY DISLOCATIONS AND GRAIN BOUNDARY DISLOCATION SOURCES BY TRANSMISSION ELECTRON MICROSCOPY — $ 66,000 — 01-1
L. E. Murr - Dept. of Metallurgical and Materials Engineering
Phone: (505)-835-5211

Characterization of ledges and arrays of dislocations in grain boundaries in Type 304 stainless steel; HVEM, in-situ observations of ledges operating in grain boundaries at low strains.

CITY UNIVERSITY OF NEW YORK, BROOKLYN COLLEGE

386. OPTICAL AND ELECTROCHEMICAL INVESTIGATION OF RUTHENIUM AND IRIDIUM OXIDES IN RELATION TO THEIR ELECTROCATALYTIC ACTIVITY — $ 67,700 — 03-3
F. Pollak - Dept. of Physics
Phone: (212)-780-5818

Studies of factors affecting behavior of Ru and Ir oxides as electrocatalysts for reduction of O_2. Determination of electronic energy levels and density of states from optical and u.v. photoemission, Raman and infrared spectroscopy.

CITY UNIVERSITY OF NEW YORK, CITY COLLEGE

387. MELTING PHENOMENA INVESTIGATED BY LASER LIGHT SCATTERING — $ 69,575 — 02-2
H. Z. Cummins - Dept. of Physics
Phone: (212)-690-6921

Brillouin scattering investigations of succinonitrile and ThCl to determine the temperature-dependent behavior of the elastic properties through the melting temperature (T^m) and impurity effects therein. Photon correlation studies of the growth of succinonitrile to assess the validity of growth models. Raman and Brillouin scattering, interferometric, and photon correlation investigations of sodium beta alumina with the goals of unambiguous separation of ionic motion and defect effects and elucidation of long-term conduction effects. Studies of anomalous thermal and mass diffusion in the melt near T^m, of zone refining of colloidal crystals, and of heterogeneous and homogeneous growth nucleation.

CITY UNIVERSITY OF NEW YORK, CITY COLLEGE (continued)

388. CRITICAL CONDITIONS FOR THE GROWTH OF SiC, Si_3N_4, and SiO_2 — $ 41,800 — 01-5
F. W. Smith - Dept. of Physics
Phone: (212)-690-6963

Critical conditions for chemical vapor deposition growth of films of SiC, Si_3N_4, and SiO_2 on single crystal Si substrate 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. Analytical techniques include electron spectroscopy for chemical analysis, Auger electron spectroscopy, secondary ion mass spectroscopy, infrared absorption, and X-ray diffraction.

STATE UNIVERSITY OF NEW YORK

389. SYNCHROTRON TOPOGRAPHIC PROJECT PARTICIPATING RESEARCH TEAM — $325,000 — 01-1
J. C. Bilello - Dept. of Materials Science and Engineering
Phone: (516)-246-6150
J. M. Liu - 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.

STATE UNIVERSITY OF NEW YORK/BINGHAMTON

390. ENERGIES AND BONDING IN MANGANESE PHOSPHIDES — $ 36,000 — 03-3
C. E. Myers - Dept. of Chemistry
Phone: (607)-798-2269

Synthesis and thermodynamic constants of members of the Mn-P system. Dissociation pressure measurements by mass-loss effusion and mass spectrometry; similar measurements on the Ni-P system.

STATE UNIVERSITY OF NEW YORK/STONY BROOK

391. CONSTRUCTION AND MAINTENANCE OF SUNY FACILITIES AT THE NATIONAL SYNCHROTRON LIGHT SOURCE — $250,000 (14 months) — 02-2

J. Bigeleisen - Vice President for Research
Phone: (516)-246-7945

Development of an X-ray beam line at NSLS for a Participating Research Team (PRT) with members from SUNY campuses at Albany, Buffalo, Stony Brook, and Cortland, and from NBS and RPI. Line will include facilities for high-resolution crystallography, surface science, XPS, small-angle X-ray scattering, and EXAFS together with capabilities for sample preparation, environmental control, and data handling. Research program will be multi-faceted with an emphasis on surface science and crystallography.

392. SURFACE STUDIES: A PROPOSAL FOR A PARTICIPATING RESEARCH TEAM AT NSLS — $250,000 (10 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.

393. THEORETICAL STUDIES OF CHEMISORPTION OF TRANSITION METAL SURFACES: INTERACTION OF HYDROGEN WITH TITANIUM — $179,300 (2 years) — 02-3

J. L. Whitten - Dept. of Chemistry
Phone: (516)-246-6068/5050
J. D. Doll - Dept. of Chemistry
Phone: (516)-246-5014/5050

Theory of chemisorption of atoms and molecules on solid surfaces: development of a general, cluster formalism and applications to H and H_2 adsorption on both flat and stepped close-packed Ti surfaces, to H_2 adorption on other Ti surfaces, and to CO adsorption on Ti (0001). Dissociative adsorption of H_2 on Ti. Objectives are an ab initio formalism for treating electronic interactions when both localized and delocalized interactions occur and a general description of surface-region bonding, which includes the response of the lattice to the adsorbate.

NORTH CAROLINA STATE UNIVERSITY

394. DEVELOPMENT OF AN X-RAY BEAM LINE AT THE NSLS FOR STUDIES IN MATERIAL SCIENCE USING X-RAY ABSORPTION — $520,000 (14 months) — 02-2

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

Development of an advanced 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 to ∿20 keV and include provisions for transmission EXAFS, fluorescence EXAFS, SEXAFS, and X-ray absorption studies other than those associated with EXAFS. Wide-ranging materials science research program: metallurgy, corrosion, amorphous materials, catalysis, surface science, electrochemistry, magnetic properties.

UNIVERSITY OF NORTH CAROLINA

395. THE STRUCTURE OF NEUTRON DAMAGE IN IONIC REFRACTORY OXIDES — $ 48,742 — 01-4

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

Structure, thermal stability, and influence of charge state upon the behavior of lattice defects created by particle 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, $MgAl_2O_4$, $Y_3Al_5O_{12}$, and TiO_2.

NORTHEASTERN UNIVERSITY

396. HIGH PRESSURE STUDIES TO DETERMINE THE EFFECTS OF VOLUME AND TEMPERATURE ON THE LATTICE DYNAMICS OF MOLECULAR SOLIDS — $ 40,056 — 02-2

F. D. Medina - Dept. of Physics
Phone: (617)-437-2918

High pressure (up to 10 Kbar) spectroscopic (Raman, infrared, neutron scattering at BNL) studies to determine the effects of volume, and temperature on the lattice dynamics of molecular solids (N_2, CO_2, and CH_4). The goal of this research is to provide additional information on the volume dependencies and anharmonicities of the intermolecular potentials in these materials.

NORTHEASTERN UNIVERSITY (continued)

397. EQUILIBRIUM AND TRANSPORT PROPERTIES OF DISORDERED TRANSITION AND NOBLE METAL ALLOYS — $104,998 (two years) — 02-3

P. N. Argyres - Dept. of Physics
Phone: (617)-437-2924
A. Bansil - Dept. of Physics
Phone: (617)-437-2923

Theoretical studies of equilibrium and transport properties of disordered metals, in particular, transition and noble metal alloys and transition metal hydrides. Theoretical framework is the coherent potential and average t-matrix approximations, with realistic muffin-tin potentials; equilibrium and transport properties are approached in a unified fashion. Specific problems include noble metals containing polyvalent solutes, noble and transition metal alloys involving two d bands, and Pd-H.

398. STUDIES OF METAL-SEMICONDUCTOR INTERFACES IN CATALYSIS AND ENERGY CONVERSION — $ 76,000 — 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.

399. EFFECT ON POINT DEFECTS ON MECHANICAL PROPERTIES OF METALS — $ 72,000 — 01-2

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

Experimental and analytical investigation of coating-enhanced ductility of Nb at low temperatures; changes in deformation mechanism, i.e., primary vs anomalous slip, with specimen orientation and with coatings; H_2 charging effects on deformation and fracture of Fe.

NORTHWESTERN UNIVERSITY (continued)

400. INVESTIGATION OF DISPERSED IRON ALLOY CATALYSTS IN THE CARBON MONOXIDE-HYDROGEN SYNTHESIS REACTION — $ 94,000 — 01-3

J. B. Butt - Dept. of Chemical Engineering and Materials Science
Phone: (312)-492-7620
L. H. Schwartz - Dept. of Chemical Engineering and Materials Science
Phone: (312)-492-5370

Preparation and characterization of Fe binary alloy catalysts useful in the CO_2-H_2 synthesis; identification of particle sizes and phases formed in the catalyst upon preparation, calcination; reduction and carburization; transmission electron microscopy, X-ray diffraction, Mossbauer spectroscopy; Fe-Ni, Fe-N, Fe-Ru, Fe-Os materials.

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

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

Investigation of factors affecting electronic and mass transport behavior in solid electrolyte and electrode materials; study of the effect of a dispersed second (non-soluble) phase on ionic transport in solid electrolytes; synthesis and characterization of new materials which are potential candidates for solid electrodes or electrolytes in energy storage or conversion devices; and optimization of the factors affecting the fabrication and ion transport properties of dense polycrystalline specimens of new solid electrolyte and electrode materials. Experimental effort involves measurements of ac conductivity, dc polarization, tracer diffusion, dielectric loss, and ion thermal current. Experimental techniques include Raman spectroscopy, NMR line-narrowing, and the chemical preparation and crystal growth of selected electrolyte materials. Materials under investigation include layered structures β" aluminas and β" gallates in which mobile cation motion is constrained to two dimensions and intersecting tunnel structures (NASICON and sodium antimonate which allow migration of the mobile alkali ion specie in three-dimensionally-linked interstitial space).

NORTHWESTERN UNIVERSITY (continued)

402. INVESTIGATION OF DEEP LEVEL DEFECTS IN EPITAXIAL SEMI-CONDUCTING ZINC SULPHO-SELENIDE — $ 47,000 — 01-3

B. W. Wessels - Dept. of Materials Science and Engineering
Phone: (312)-492-3536

Preparation of high purity ZnS_xSi_{1-x} heteroepitaxially deposited by chemical vapor deposition on substrates of ZnSe, GaAs, and Ge. Defect identification and exploration of compensation mechanisms by measuring ionization energies of deep acceptors and donors using deep level transient spectroscopy on deliberately doped n-type and p-type material. Role of misfit dislocations on deep level defects.

UNIVERSITY OF NOTRE DAME

403. PORE SHRINKAGE AND OSTWALD RIPENING IN METALLIC SYSTEMS — $ 56,000 — 01-1

G. C. Kuczynski - Dept. of Metallurgical Engineering and Materials Science
Phone: (219)-283-6151
C. W. Allen - Dept. of Metallurgical Engineering and Materials Science
Phone: (219)-283-6198

General theory of Ostwald ripening of pores and voids in sintered compacts of Ni_3Al and in Ni_3Al containing voids produced by high energy electron and ion bombardment; Ostwald ripening of precipitates in solid matrices. High voltage and scanning transmission electron microscopy.

OHIO STATE UNIVERSITY

404. ELECTRICAL TRANSPORT AND OPTICAL PROPERTIES OF RANDOM SMALL PARTICLE COMPOSITES — $109,376 — 02-2

J. C. Garland - Dept. of Physics
Phone: (614)-422-7277
D. B. Tanner - Dept. of Physics
Phone: (614)-422-7855

This is a program of experimental research on the electrical transport and optical properties of a new model composite material. The material is a dielectric medium with small metal particles randomly distributed throughout. Critical phenomena associated with percolation and the dynamics of granular superconductors are two principal interests.

OHIO STATE UNIVERSITY (continued)

405. FUNDAMENTAL STUDIES OF HIGH TEMPERATURE CORROSION REACTIONS — $ 98,000 — 01-1
R. A. Rapp - Dept. of Metallurgical Engineering
Phone: (614)-422-6178

In-situ SEM study of oxidation of metals, initially Cu and Ni-Cr alloys; oxide nucleation and growth; scale cracking and healing; mechanisms and kinetics of sulfidation of Mo; scale structure and epitaxy with substrate.

406. HYDROGEN ATTACK OF STEEL — $ 44,873 — 01-2
P. G. Shewmon - Dept. of Metallurgical Engineering
Phone: (614)-422-2491

Atomic processes of hydrogen attack of pressure vessel steels; high hydrogen pressures and relatively high temperature; decarbonization, methane bubble formation and cracking/fissue formation; high-sensitivity dilatometry, scanning electron microscopy and scanning Auger spectroscopy; effects of deoxidation practice; carbon activity measurements.

OKLAHOMA STATE UNIVERSITY

407. ELECTRONIC STRUCTURE OF DEFECTS IN OXIDES — $ 29,300 (2 years) — 02-2

G. P. Summers - Dept. of Physics
Phone: (404)-624-5813

Photoconductivity and fluoroescence measurements in oxides --α-Al_2O_3 and SrO; determination of electronic structure of defects and changes produced by γ-ray, electron, neutron or proton irradiation; effect of V, Cr, and Fe impurities on charge transfer in α-Al_2O_3.

UNIVERSITY OF OREGON

408. THE ELECTRICAL STRUCTURE OF SEMICONDUCTORS AND METALS — $ 48,183 — 02-3

James R. Chelikowsky - Dept. of Physics
Phone: (503)-686-4725/5204

Recently developed theoretical techniques will be used to investigate the properties of electronic surface structure, the theory of angle resolved photoemission spectroscopy, and the temperature and pressure dependence of band gaps, charge densities and X-ray form factors in semiconductors. Theoretical studies will be initiated to find a microscopic explanation for the empirical schemes which predict structural energies and heats of formation of intermetallic alloys. This latter will be done by the direct calculation of the cohesive energy of alloys.

PENNSYLVANIA STATE UNIVERSITY — $ 40,000 — 01-2

409. SUPERPLASTICITY AND FRACTURE OF CERAMICS

R. C. Bradt - Dept. of Materials Science
Phone: (814)-865-4631

Superplastic deformation during phase transitions in ceramic systems and the effects of structure and microstructure on fracture in ceramic systems. Transformational superplasticity in Bi_2O_3, the Bi_2O_3-Sm_2O_3 eutectoid, Bi_2WO_6 and Bi_2MoO_6. Investigation of transitions in R_2O_3-(WO_3MoO_3), where R_2O_3 is a rare earth oxide with an emphasis on the $\Delta V/V$ of the phase transitions. Stoichiometry effects on fracture in TiO_{2-x} and $Fe_{1-x}O$. Fracture in single crystal and polycrystalline $MgAl_2O_4$ and $MgO \cdot XAl_2O_3$. Structural, temperature, and irradiation effects on the fracture process in CaF_2.

410. PHYSICAL ADSORPTION: RARE GAS ATOMS NEAR SOLID SURFACES — $ 44,153 — 02-2

M. W. Cole - Dept. of Physics
Phone: (814)-863-0165/7533

Theory of the interaction between an incident atomic or molecular beam and a surface: inelastic effects in the scattering of He from graphite and alkali halides; scattering of H_2 from graphite; scattering of molecules and atoms from diamond, layer compounds, and adsorbed layers. Theory of the physisorption potential: validity of additivity of adatom-substrate atom interactions for He on graphite; interaction between other rare-gases and graphite; analysis of disparity between potentials from ab initio calculations and those obtained from scattering data. Thermodynamics and statistical mechanics of He films of various thicknesses on graphite. Theory of photostimulated field emission, with and without adsorbates.

411. HYDROGEN ABSORPTION IN METALS: A FIELD ION MICROSCOPY STUDY — $ 57,000 — 01-1

H. W. Pickering - Dept. of Materials Sciences & Engineering
Phone: (814)-865-5446
T. Sakurai - Dept. of Physics
Phone: (814)-863-2115

Field ion microscopy study of H_2 trapping and absorption in Fe; also oxide formation as well as Ti-O clustering and segregation at grain boundaries; surface and grain boundary segregation of solutes (Sn, Sb, others) in Ni and Fe.

412. GRAIN BOUNDARY DIFFUSION AND GRAIN BOUNDARY CHEMISTRY OF CR-DOPED MAGNESIUM OXIDE — $ 35,000 — 01-3

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

Grain boundary diffusion and characterization in ceramics, initially Cr-doped MgO; effect of boundary composition; techniques used: radioactive tracers, autoradiography, TEM, ion beam spectrochemical analysis; electron microprobe.

413. STRUCTURE OF GLASSES CONTAINING TRANSITION METAL IONS — $ 88,000 — 01-1

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

Structure and properties of insulator glasses and the same glasses containing transition metals. The structure is determined on silicate, alumino-silicate and boro-silicate glasses primarily by Raman and infrared spectroscopy. Investigation of local environment of the transition metal ions by optical absorption, luminescence, and Raman spectroscopy. Crystallization and the thermodynamics of metal reduction from melts are investigated to provide information on the structure of the glass. Surface processes and hydrogen diffusion into glasses are probed with sputter-induced photon spectrometry (SIPS).

UNIVERSITY OF PENNSYLVANIA

414. HIGH CONDUCTIVITY PROTON SOLID ELECTROLYTES — $ 73,000 — 03-1

G. C. Farrington - Dept. of Materials Science and Engineering
Phone: (215)-243-6642

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.

415. STUDIES RELATING TO THE HIGH CONDUCTIVITY OF INTERCALATED GRAPHITE — $112,399 — 02-2

J. E. Fischer - Dept. of Electrical Engineering and Sciences
Phone: (215)-243-6924

Synthesize various stages of Ba-intercalated graphite, particularly the stage one material BaC_6. Obtain the chemical structures of these materials, determine the stoichiometries, measure the conductivites and optical properties, and interpret the results in terms of structure and bonding properties. Prepare graphite intercalation compounds using intercalates having a wide range of fluorinating strength (XeF_6, XeF_4, AsF_5, $XeOF_4$, XeF_2). Determine the chemical character and physical properties of these compounds using a number of techniques (NMR, XPS, IR spectroscopy, Raman scattering, paramagnetic resonance, and optical spectroscopy).

416. MECHANISMS OF DAMAGE ACCUMULATION IN TIME DEPENDENT CYCLIC DEFORMATION — $ 47,200 — 01-2

Campbell Laird - Dept. of Metallurgy and Materials Science
Phone: (215)-243-8337

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; technique used - TEM.

417. SURFACE (e,2e) SCATTERING: A SURFACE STRUCTURE TOOL — $ 32,770 — 02-2

Ward E. Plummer - Dept. of Physics
Phone: (215)-243-8157

The objectives of this one year program are to design and assemble an apparatus to measure the extended fine structure in the spectrum of electrons inelastically scattered from the surface of model materials. In order to discriminate against background radiation, the inelastically scattered electrons will be measured in coincidence with other electrons produced in the inelastic scattering event, either directly or by Auger processes. Measurements will be made on model substances such as oxygen on surfaces of single crystal nickel.

418. ATOMISTIC STUDIES OF GRAIN BOUNDARIES WITH SEGREGATED IMPURITIES — $ 50,100 — 01-1

V. Vitek - Dept. of Metallurgy and Materials Science
Phone: (215)-243-7883

Atomistic-based computer simulation of grain boundary structure in dilute 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.

419. ELECTROCHEMICAL INVESTIGATION OF NOVEL ELECTRODE MATERIALS — $ 99,000 — 03-2

W. L. Worrell - Dept. of Materials Science and Engineering
Phone: (215)-243-8592

Intercalation of Na and Li into Li_xTiS_2 and Li_xTaS_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.

PRINCETON UNIVERSITY

420. CHEMICAL POISONING IN HETEROGENEOUSLY CATALYZED REACTIONS — $ 60,000 — 03-1
S. L. Bernasek - Dept. of Chemistry
Phone: (609)-452-4986

LEED studies of clean Mo and adsorbed poison overlayers. Rapid scan instrumentation using Vidicon camera has been applied to collection of data for N_2, thiophene and COS overlayers on Mo (100) planes. Structural analysis of clean Co surface, and composition studies of transient surfaces showing selective displacement of one species (e.g. COS) by another (e.g. HCOOH) as a function of surface temperature and species exposure.

PURDUE UNIVERSITY

421. FORMATION OF A PARTICIPATING RESEARCH TEAM AND THE INSTRUMENTATION FOR X-RAY DIFFRACTION AT THE NATIONAL SYNCHROTRON LIGHT SOURCE — $346,400 — 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: catalysts, dilute metal alloys, non-stoichiometric oxides, intermetallic compounds, plastically deformed region ahead of stable crack, among others.

422. STUDY OF ELECTRONS PHOTO-EMITTED FROM FIELD EMISSION TIPS — $ 60,394 — 01-3
R. Reifenberger - Dept. of Physics
Phone: (317)-493-9318

Investigation of photo-induced field emitted electrons using a tunable cw dye laser. Energy resolved measurements of photo-field emitted electrons by means of a differential energy analyzer. Thermally activated surface diffusion of adatoms on a field emission tip. Thermally-induced and laser-induced chemical reactions on small metallic surfaces.

PURDUE UNIVERSITY (continued)

423. MECHANISMS OF ELEVATED TEMPERATURE RUPTURE IN SINGLE PHASE CERAMICS — $ 82,000 (11 months) — 01-3

A. A. Solomon - Dept. of Nuclear Engineering
Phone: (317)-494-7910

Study of elevated temperature stress rupture in well-characterized single phase ceramics in terms of rate controlling mechanisms and microstructural evolution. Experimental techniques consist of (1) tensile creep using constant 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, (3) characterization of initial powder, and (4) dislocation etch pitting. Preliminary studies will be on ZnO and a metallic system, followed by comprehensive studies on a stoichiometric oxide such as MgO or Al_2O_3, and a non-stoichiometric system such as CoO.

RENSSELAER POLYTECHNIC INSTITUTE

424. CHEMICAL DIFFUSION ON SOLID SURFACES — $ 39,400 — 01-3

J. B. Hudson - Dept. of Materials Engineering
Phone: (518)-270-6451

Measurement of rates of migration of adsorbates on Ni; electron stimulated desorption of NH_3 to form an N_2 adsorbate; H_2 chemisorption; techniques used - AES, mass spectrometry.

425. THERMOPHYSICAL PROPERTIES OF INORGANIC POLYSULFIDES — $ 77,100 — 03-2

G. J. Janz - Dept. of Chemistry
Phone: (518)-270-6344

Synthesis of sodium polysulfides and measurements of their enthalpies of fusion, heat capacities, and volume changes on melting. Investigations of the phase-diagram of the Na-S system.

426. PROTECTIVE OXIDE FILMS — $ 70,000 — 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 films of the protective metal oxides NiO, Al_2O_3, and Cr_2O_3 by both discontinuous and continuous thermogravimetric analysis, thermally stimulated currents, thermoluminescence, and electron paramagnetic resonance, for the purpose of obtaining a more precise understanding of the oxidation process.

RENSSELAER POLYTECHNIC INSTITUTE

427. FATIGUE BEHAVIOR OF BCC METALS — $ 38,750 — 01-2
N. S. Stoloff - Dept. of Materials Engineering
Phone: (518)-270-6495

Fatigue and delayed failure behavior of polycrystalline V and Nb. Fatigue test variables include stress level, temperature, environment, and the ratio of minimum to maximum stress. Delayed failure experiment variables include H content and critical stress level.

428. PROPERTIES OF GLASS WITH HIGH WATER CONTENT — $ 79,000 — 01-3
M. Tomozawa - Dept. of Materials Engineering
Phone: (518)-270-6477
E. Bruce Watson - Dept. of Geology
Phone: (518)-270-6477

The effects of dissolved water upon physical, chemical, and transport properties of select glass compositions containing up to ∿9 wt. % water is to be explored. These unusual high water content glasses will be prepared under combined pressure-temperature conditions of 3 kbar and 800°C. Radiation effects, chemical durability, diffusion, mechanical strength, ion transport processes, differential thermal analysis, thermogravimetric analysis.

429. LOCALIZED CORROSION AND STRESS CORROSION CRACKING BEHAVIOR OF AUSTENITIC STAINLESS STEEL WELDMENTS CONTAINING RETAINED FERRITE — $ 93,540 — 01-1
W. F. Savage - Materials Engineering Dept.
Phone: (518)-270-6453
D. J. Duquette - Materials Engineering Dept.
Phone: (518)-270-6448

Corrosion behavior of stainless steels containing welds and stainless steel weldments with particular attention to pitting and stress corrosion cracking in chloride containing solutions; variables studied include pH, chloride concentration, and welding parameters; potentiodynamic and galvanokinetic test procedures coupled with optical, electron and analytical electron microscopy; stress corrosion cracking at slow strain rates in pressure vessles with electrochemical monitoring of potentials.

UNIVERSITY OF ROCHESTER

430. THE MATERIALS AND MECHANICS OF RATE EFFECTS IN BRITTLE FRACTURE — $ 65,308 — 01-2

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

Analytical and experimental studies of brittle fracture; thermodynamic (state variable) description of fracture processes; double torsion and double contilever beam test techniques; slow and fast crack growth rates versus crack driving force at various temperatures; brittle plastic PMMA, mild steels, LiF; fatigue studies in LiF.

431. DIFFUSIONAL CREEP OF MULTI-COMPONENT SYSTEMS — $ 69,276 — 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, polymeric 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 and diffusion; Al, β-tin, LiF, KBr, PMMA, rubber.

ROCKWELL INTERNATIONAL SCIENCE CENTER

432. ACOUSTIC EMISSION SIGNATURE ANALYSIS — $ 94,038 — 01-5

O. Buck - Science Center
Phone: (805)-498-4545

Application of acoustic emission to detection of cracking mechanisms in glass and metals; crack growth in embrittled steels; sustained load cracking of hydrogen embrittled steel; multiple transducer Fourier frequency analysis of acoustic emissions; fracture momentum concept. Acoustic emission analysis as a function of geometric parameters and of fatigue-crack growth.

433. SINTERING PHENOMENA OF NON-OXIDE SILICON COMPOUNDS — $ 89,995 — 01-1

D. R. Clarke
Phone: (805)-498-4545
F. F. Lange
Phone: (805)-498-4545

Studies to understand the volatilization phenomenon associated with non-oxide silicon compounds which presently inhibits the sinterability of single phase powders and hinders densification with a sintering aid, and studies to understand the liquid phase sintering phenomena associated with non-oxide silicon compounds containing a sintering aid. The overall goal is to understand the interrelation between phase equilibria and fabrication parameters, with emphasis on Si_3N_4 and SiC systems. Si_3N_4-SiO_2-Y_2O_3 phase equilibria. Diffusion. Scanning transmission electron microscopy. Analytical electron microscopy.

SERI/UNIVERSITY PROGRAMS

434. Solar Energy Research Institute - University Programs
A. Kotch - SERI - Phone: (303) 231-1823

University programs funded through SERI:

University of Vermont (R. L. Anderson) "Influence of the Interfacial Layer on Electrooptical Properties of Heterojunction Solar Cells"	$ 63,951
University of Missouri-Rolla (J. L. Boone, T. Van Doren) "Investigation of Chemical Spray Techniques for the Growth of Thin Film CdTe Solar Cell Materials"	$ 72,175
University of Maine-Orono (A. H. Clark) "Growth and Characterization of Ternary Semiconductor Compounds Produced by Molecular Beam Epitaxy"	$ 67,357
University of Delaware (E. A. Fagen) "Transport Properties of Amorphous Silicon-Germanium Alloy Films"	$ 78,848
Brown University (H. J. Gerritsen, A. V. Nurmikko) "Characterization of Photovoltaic Interfaces by Picosecond Optical Methods"	$ 85,505
North Carolina State University (K. W. Hanck, A. F. Schreiner, M. A. Littlejohn) "Electrodeposition of Semiconductors and Photovoltaic Solar Cells"	$ 81,000
University of Florida (P. H. Holloway) "Kinetics and Mechanisms of Degradation of Metal Black Selective Solar Absorber Coatings"	$ 51,164

UNIVERSITY OF SOUTHERN CALIFORNIA

435. ELECTRICAL AND MECHANICAL PROPERTIES OF OXIDE CERAMICS — $ 71,500 — 01-3
F. A. Kröger - Electronic Sciences Laboratory
Phone: (213)-741-6224

Electrical conductivity, transference number, and creep rate as a function of oxygen pressure, dopant concentration, temperature, and grain size in MgO and Al_2O_3 with emphasis on the delineation between grain boundary and bulk effects, and on the determination of the relation between composition, conditions of sample preparation, and physical behavior.

436. GRAIN BOUNDARY SLIDING AND DEFORMATION MECHANISMS DURING HIGH TEMPERATURE CREEP — $ 95,000 — 01-2
T. G. Langdon - Dept. of Materials Science and Mechanical Engineering
Phone: (213)-741-2095

Measurement of creep and grain boundary sliding in metals--Al, Mg, and Cu, and their alloys--and in alkali halides--KBr; boundary sliding, stress and temperature dependences, threshold creep stress in precipitation hardened alloys; identification of dominant deformation mechanisms; effect of crystallographic orientation on transient creep of KBr; deformation and fracture map construction.

437. EVAPORATION DRIVEN LIQUID SINTERING — $ 45,700 — 01-1
J. W. Whelan - Dpt. of Materials Sciences
Phone: (213)-741-6219

Reaction driven liquid sintering in which the liquid sintering aid is extracted into a second phase. Processes occurring during permeation annealing and evaporative annealing of cold pressed MgO-LiF compacts. Final stage sintering in the SiC-Si system with the objectives of removing the residual Si and leaving behind SiC of near theoretical density and clean grain boundaries. Sintering in the Si_3N_4-Si system.

SOUTHWEST RESEARCH INSTITUTE

438. THE STUDY AND MODELLING OF HIGH TEMPERATURE FATIGUE CRACK PROPAGATION IN AUSTENITIC STAINLESS STEEL — $ 61,000 — 01-2
D. L. Davidson - Dept. of Materials Sciences
Phone: (512)-684-5111

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

STANFORD UNIVERSITY

439. PHOTOELECTRONIC PROPERTIES OF II-VI HETEROJUNCTIONS — $144,579 — 01-3

R. H. Bube - Dept. of Materials Sciences 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; spectral response; diffusion lengths; scanning transmission electron microscopy analysis of heterojunction interfaces; lattice resolution; electron microdiffraction; vacuum evaporation; spray pyrolysis; rf sputter deposition.

440. EXCITED STATE ENERGY TRANSPORT IN SOLUTIONS AND AMORPHOUS MATERIALS — $ 76,000 — 03-1

M. D. Fayer - Dept. of Chemistry
Phone: (415)-497-4446

Picosecond laser measurements of the transfer of electronic excitation in solutions of Rhodamine 6G. Theoretical and experimental studies of mechanism of energy transport in amorphous materials. A major aim of the program is to develop a basic understanding of the optical and chemical properties necessary for the development of artificial photosynthesis.

441. SUPERCONDUCTING AND SEMICONDUCTING PROPERTIES OF ELECTRON BEAM EVAPORATED MATERIALS — $130,000 — 02-2

T. H. Geballe - W. W. Hansen Laboratories of Physics
Phone: (415)-497-0215
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, as well as other mechanical properties such as strain tolerance, micro-hardness and high temperature ductility are studied as a function of composition and microstructure.

STANFORD UNIVERSITY (continued)

442. MODELLING OF DEFORMATION AND FRACTURE IN HIGH-TEMPERATURE STRUCTURAL MATERIALS — $130,000 — 01-2

A. K. Miller - Dept. of Materials Science and Engineering
Phone: (415)-497-3732
O. D. Sherby - Dept. of Materials Science and Engineering
Phone: (415)-497-2536

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"; interactive solute strengthening in Type 316 stainless steel; roles of forest dislocations and subgrains in isotropic hardening, Type 304 stainless steel; back stresses at large strains and high temperatures, Al and Type 304 stainless steel; strain softening; application of MATMOD equations to 2 1/4 Cr-1Mo steel; elevated temperature fatigue with hold time in ferritic materials.

443. MECHANISMS AND MECHANICS OF HIGH TEMPERATURE FRACTURE OF MATERIALS — $ 80,600 — 01-2

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

Analytical and experimental investigation of creep rupture in metals - Cu and Ag; effects of grain boundary segregation, e.g., O in Cu, and arrays of cavities (H_2O bubbles) at boundaries; cavity nucleation and growth kinetics and energetics; rupture time modelling considering both surface and boundary diffusion; technique used: Auger electron spectroscopy.

444. DIFFUSION OF OXYGEN IN LIQUID METAL SYSTEMS — $ 39,184 — 01-3

D. A. Stevenson - Dept. of Materials Science and Engineering
Phone: (415)-497-4251

Influence of composition, preparation, and high temperature annealing upon the total and partial conductivities and on the microstructure of yttria-stabilized zirconia oxygen solid electrolytes. a.c. conductivity and complex admittance analysis to separate out bulk and grain boundary effects. Ordering and grain boundary microchemistry studies by STEM analytical techniques.

SYRACUSE UNIVERSITY

445. SURFACE CHARACTERIZATION OF CATALYTICALLY ACTIVE METAL ALLOY AND COMPOUND FILMS — $ 90,000 — 01-1

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

Defect structure of thin metal films (Ag/Cu, Pd/Cu, Pt/Cu); interfacial dislocations; overgrowth structure and growth mechanisms; techniques used TEM, AES, RHEED.

UNIVERSITY OF TENNESSEE

446. A COMBINED THERMODYNAMIC STUDY OF NICKEL BASE ALLOYS — $ 75,000 — 01-1

C. R. Brooks - Dept. of Chemical and Metallurgical Engineering
Phone: (615)-974-5427
P. J. Meschter - Dept. of Chemical and Metallurgical Engineering
Phone: (615)-974-6009

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

447. MODELING OF ULTRASONIC NON-DESTRUCTIVE EVALUATION OF COLUMNAR STRUCTURES IN ANISOTROPIC MATERIALS — $ 90,000 — 01-5

L. Adler - Nondestructive Evaluation Division
Phone: (615)-974-3342
B. Dewey - Nondestructive Evaluation Division
Phone: (615)-974-3342
B. Oliver - Nondestructive Evaluation Division
Phone: (615)-974-3342

Ultrasonic measurements of elastic constants on single crystals of Ni and Ni based alloys; finite element solutions to the ultrasonic wave propagation; single crystal model to be extended to bicrystals; transmission and reflection coefficients of the interface to be determined as a function of frequency and angle.

UNIVERSITY OF UTAH

448. IMPURITY EFFECTS ON THE CREEP OF POLYCRYSTALLINE MAGNESIUM AND ALUMINUM OXIDES AT ELEVATED TEMPERATURES — $ 14,180 — 01-2

R. S. Gordon - Materials Science and Engineering Division
Phone: (801)-581-6612

Effects of temperature (1100-1500°C), grain size (10-100μm) and stress (1-100MN/m^2) on the creep and/or stress relaxation of polycrystalline aluminum and/or magnesium oxides doped simultaneously or individually with Mn, Ti, and Fe in amounts between 0.2 and 3.0 cation % total impurities. Concerns include: (1) The effect of mixed dopants on the creep of polycrystalline Al_2O_3, (2) Stress relaxation deformation studies on pure and doped, polycrystalline Al_2O_3 and MgO, and (3) Construction of creep deformation maps for pure and doped, polycrystalline MgO and Al_2O_3.

449. THE EFFECT OF PROCESSING CONDITIONS ON THE RELIABILITY OF CROSS-LINKED POLYETHYLENE CABLE INSULATION — $ 77,235 — 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 semiconducting layer. Morphology, dielectric loss spectra and treeing properties of an extensive series of miniature cables will be determined under carefully controlled extrusion, cross-linking and crystallization conditions. Apparatus for accelerated testing of "treeing" is under construction.

450. ELECTROLYTIC DEGRADATION OF LITHIA-STABILIZED β" ALUMINA — $ 80,000 — 03-2

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

Studies of degradation of β-alumina near the melting point of Na, including effects of local enhancement of 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.

VIRGINIA POLYTECHNIC INSTITUTE
AND STATE UNIVERSITY

451. HYDROGEN EMBRITTLEMENT TESTING — $ 30,000 — 01-2
M. R. Louthan, Jr. - Dept. of Materials Engineering
Phone: (703)-961-6640

Evaluation of the effective hydrogen 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.

UNIVERSITY OF VIRGINIA

452. SPECTROSCOPY OF SURFACE ADSORBED MOLECULES — $ 90,490 — 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), photoemission (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 interactions between molecules and interface. ESCA and Auger studies will be made on the same systems to augment the IETS work. Studies of UV-induced damage to molecules and photocatalytic effects on semiconductor oxides.

WASHINGTON UNIVERSITY

453. MICROSCOPIC DETERMINATIONS OF LATTICE AND ELECTRONIC STRUCTURES OF SOLIDS — $ 67,256 — 02-2
P. C. Gibbons - Dept. of Physics
Phone: (314)-889 6271

High-energy electron energy-loss spectroscopy: physical processes influencing core-electron threshold behavior with emphasis on Mg and Al in insulating, semiconducting, and metallic solids; generalized oscillator strengths and exciton effects. EXAFS investigations: momentum-transfer dependence of EXAFS spectra; structural studies with Al, Si, C, O, N, and Fe in various materials; relations between the properties of macromolecules and local structure in the vicinity of heavy atoms; studies of hydrogen residence sites, residence times, and hopping rates in hydrogen-bearing metals; structure of amorphous Si. Instrument capabilities are such that many of these investigations can be done with micron-sized samples.

UNIVERSITY OF WASHINGTON

454. NUCLEAR MAGNETIC RESONANCE STUDIES OF ION MOTION IN SOLID ELECTROLYTES — $ 58,000 — 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 times, effects of motion and structure upon the dielectric quadrupole NMR spectrum, and direct NMR diffusion measurements to study the solid electrolytes mixed cation β-alumina and alkali containing borate glasses. Correlative studies involve electrical conductivity and thermal analysis. Temperature and frequency dependence of the spin-lattice relaxation to understand ion-ion and ion-lattice interactions and predict electrolyte systems with optimized conductivity.

UNIVERSITY OF WISCONSIN, MADISON

455. LOCAL ELECTRONIC PROPERTIES OF SEMICONDUCTOR SURFACES AND INTERFACES — $ 94,913 — 02-2

M. G. Lagally - Dept. of Metallurgical and Mineral Engineering
Phone: (608)-263-2078

Correlations will be made between site-specific electronic properties and surface structure for compound semiconductors such as GeS, GeSe, SnS, SnSe, GaS, GaSe, GaTe, MoS_2, CdS, CdSe, CdTe and intermetallic compounds such as InSn, InPb, CdCu and CdMg. Some ternary systems such as $GaSe_{1-x}S_x$ and $SnSe_{2(1-x)}S_{2x}$ will also be studied. Techniques used include LEED, AES, XPS, UPS, and electron stimulated disorption. The second part of the proposed research deals with detailed structural and chemical analysis of thin epitaxial films and interfaces between these films and substrates. Initial studies will be on Ge films deposited on GeS or GeSe. LEED, AES and XPS line widths will be measured as a function of film thickness.

456. ELECTRONIC STRUCTURE STUDIES OF METAL-HYDROGEN SYSTEMS USING PHOTOELECTRON SPECTROSCOPY (PES) RADIATION — $164,159 — 02-2

J. H. Weaver - Physical Sciences Laboratory
Phone: (608)-873-6651

The principal investigator intends to use photoelectron spectroscopy (PES) to study the electronic structure of several metal hydrides in order to better understand their properties as hydrogen storage materials. During the first year preliminary studies will be made on Nb_4D_3 and Ta_2D. Possible temperature dependencies and the effects of different surface conditions on PES for the α phase of ScH_x and YH_x will be examined. There will also be a study of the metal to semiconductor transition in Lanthanum series metal hydrides. In addition, the principal investigator intends to construct and assemble the equipment necessary for angle resolved PES. When the apparatus is completed angle resolved PES measurements will be made on NB_4D_3 and other single crystals.

UNIVERSITY OF WISCONSIN, MADISON (continued)

457. PREDICTION OF THE BEHAVIOR OF STRUCTURAL MATERIALS UNDER IRRADIATION THROUGH MODELLING OF THE MICROSTRUCTURE — $ 35,000 — 01-4

W. G. Wolfer - Dept. of Nuclear Engineering
Phone: (608)-263-6818

Modelling irradiation-induced void and dislocation loop nucleation and growth as stochastic clustering processes; effect of coatings on void-interstitial and void-vacancy interactions; formation of dislocation network; evaluation of irradiation - enhanced creep models and crystallographic orientation effects thereon; measurement of cumulative creep damage under biaxial stresses.

UNIVERSITY OF WISCONSIN, MILWAUKEE

458. INTERACTION OF LOW ENERGY ELECTRONS WITH SURFACE LATTICE VIBRATIONS — $ 51,806 — 02-2

S. Y. Tong - Dept. of Physics
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.

SECTION C

Summary of Funding Levels

The summary funding levels for various research categories were determined from the index listing in Section D and estimating the percentage from the project devoted to a particular subject. There is overlap in the figures. For instance, funding for a project on 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, 1979, the Materials Sciences total support level amounted to about $78.4 million in operating funds (budget outlays) and $6.3 million in equipment funds. The equipment funds are expended primarily at Laboratories and are not shown in this analysis. Equipment funds for the University 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	19.5
(b) South ..... (Fla., N.C., Tenn., Va., La., Ga.)	9.5	22.5
(c) Midwest ..... (Ohio, Ill., Wisc., Mich., Mo., Minn., Ind., Iowa, Kan.)	22.4	36.8
(d) West ..... (Ariz., Okla., Wash., Texas, N. Mex., Calif., Utah, Colo., Idaho)	22.8	21.2
	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-)	59.8	44.5

	Contract Research (% by $)	Total Program (% by $)
(b) Physics, Solid State Science, Solid State Physics (Office Budget Activity Numbers 02-)	30.6	41.7
(c) Chemistry, Chemical Eng. (Office Budget Activity Numbers 03-)	9.6	13.8
	100.0	100.0

3. By University, DOE Laboratory, and Industry:

	Total Program (% by $)
(a) Programs (including those laboratories where graduate students are involved in research to a large extent, e.g., LBL, Ames)	36.7
(b) DOE Laboratory Programs	63.3
	100.0

4. By Laboratory:

	Total Program (%)
Ames Laboratory	7.8
Argonne National Laboratory	21.6
Brookhaven National Laboratory	10.8
Idaho National Engineering Laboratory	0.6
Illinois, University of (Materials Research Laboratory)	2.8
Lawrence Berkeley Laboratory	7.0
Lawrence Livermore Laboratory	1.5
Los Alamos Scientific Laboratory	2.6
Mound Laboratory	0.3
Oak Ridge National Laboratory	20.7
Pacific Northwest Laboratory	2.2
Sandia Laboratory	2.5
Solar Energy Research Institute	0.3
Contract Research	19.3
	100.0

5. By Selected Areas of Research:

	Number of Projects (Total=392) (%)	Total Program $ (%)
(a) Materials		
Polymers	5.6	1.8
Ceramics	31.4	17.2
Semiconductors	12.5	7.9
Hydrides	8.9	5.2
Ferrous Metals	18.1	10.9
(b) Technique		
Neutron Scattering	8.7	16.5
Theory	18.6	9.0
(c) Phenomena		
Catalysis	8.4	4.9
Corrosion	9.4	13.1
Diffusion	16.1	6.6
Superconductivity	11.2	7.4
Strength	21.7	9.9
(d) Environment		
Radiation	14.0	12.5
Sulphur-Containing	5.9	3.0

Section D

Index of Investigators, Materials, Phenomena, Technique and Environment

The index refers to project numbers in Sections A & B.

Actinide Metals and Compounds

3	186
37	194
38	201
53	202
59	207
67	217
168	370

Ceramics

Carbides

50	196
66	200
67	202
69	204
100	207
106	332
121	348
149	365
175	388
188	415
191	433
194	437

Glass

37	219
43	308
67	318
83	322
107	336
156	382
157	413
158	428
202	432
215	454

Nitrides

100	336
106	348
173	363
188	365
191	376
200	382
202	388
204	433

Oxides

11	105	201	372
12	108	202	380
19	109	204	381
20	111	205	384
32	125	207	386
34	129	215	388
37	131	217	395
40	132	218	398
43	133	220	401
55	136	301	405
66	138	307	407
67	149	316	409
69	160	320	412
77	163	321	414
81	167	324	421
82	173	327	423
84	182	354	426
86	186	356	435
87	187	362	437
88	189	363	444
90	191	365	448
92	193	368	450
93	194	370	452
100	196	371	454
103	200		

Composites

14	202
23	335
57	339
75	340
130	352
173	355
185	404
191	419
200	450

Fast Ion Conductors

32	195
43	196
54	203
61	314
62	327
67	370
83	379
111	401
112	414
118	419
186	444
189	450
191	454
194	

Graphite, Carbon, and Coal

30	186
33	200
36	202
84	203
100	212
122	352
124	353
134	354
153	410
172	415
174	

Hydrides

7	68	185
21	69	186
22	76	190
25	82	194
26	92	198
27	101	200
31	110	202
38	112	350
41	116	397
59	117	427
66	122	456
67	165	

Intermetallic Compounds

10	37	66	186	323
12	39	68	190	343
15	42	70	191	353
23	45	80	192	355
24	47	91	193	373
25	53	130	194	379
26	54	173	196	403
27	59	180	199	419
31	62	182	200	441
35	64	185	202	455

Ionic Crystals

80	185	194	410
81	186	196	430
90	187	201	431
156	189	217	436
158	191	387	

Liquids & Amorphous Metals

13	83	168	203	326
30	89	169	205	341
41	91	180	210	347
47	140	186	211	387
53	141	192	214	394
55	155	194	216	413
60	156	196	302	440
70	157	200	305	
74	161	202	318	

Metals

Alkali

18	325
70	353
164	419
168	425
313	

BCC Refractory

2	70	190	200	392
4	100	191	216	399
7	101	193	319	405
21	105	194	337	427
32	117	195	343	458
41	118	196	346	
45	122	198	351	
47	123	199	375	

Metals (continued)

Ferrous

5	125	186	222	347	400
7	127	191	223	361	406
8	135	193	233	364	411
9	154	194	304	366	416
13	163	195	317	369	421
20	175	196	319	372	429
50	176	197	325	375	430
52	177	198	328	378	432
70	178	213	333	380	438
71	181	214	334	385	442
73	183	216	341	392	457
124	185	218	342	399	

MHD Materials

11	187
67	188
69	191
87	196
108	381
186	

Polymers

32	172	335	380
97	186	344	387
99	195	345	430
112	226	352	431
114	234	374	449
115	306		

Rare Earth Metals and Compounds

1	21	59	162	201
2	31	66	164	202
7	36	67	185	217
14	38	68	186	312
15	42	69	191	350
17	53	80	194	381
18	54	111	199	

Semiconductors

Acoustic Emission

67
432

Auger Electron Spectroscopy

8	152	213	372
22	158	214	375
36	177	215	388
39	181	219	392
47	194	226	406
52	199	302	424
68	200	331	443
77	209	358	452
92	212	359	455

Computer Simulation

20	62	161	199	365
30	67	168	200	382
34	89	177	205	418
40	90	189	314	442
43	127	192	322	446
46	145	194	349	
61	157	196	354	

Elastic Constants

12	198
18	344
78	345
117	447
119	450

Electron Microscopy

40	79	163	191	216	330	385
41	100	170	192	217	331	399
43	103	174	193	218	332	400
45	107	176	196	219	337	403
46	109	177	200	223	342	405
47	124	181	201	301	350	416
48	125	182	202	308	356	429
50	126	183	215	311	362	433
52	128	187	212	317	365	438
68	129	188	213	319	376	444
73	133	189	214	320	381	445
75	138	190	215	321	384	453
76	160					

Electron Spin Resonance

22	111	314
25	187	395
26	191	426
55	192	
58	201	

Field Emission and Ion Microscopy

36	337
41	384
46	410
226	411
227	422

High Temperature Heat Capacity

148
169
179
446

Infrared Spectroscopy

22	159	192	396
60	187	379	404
72	188	380	413
94	189	386	415
139	191	388	449
156			

Internal Friction

3	305
40	323
78	327
101	344
117	345
161	346
198	

Ion Channeling, Scattering and Implantation

22	181	199
46	190	200
47	192	214
48	194	223
52	196	373
88	197	394
110	198	

Laser Beam Scattering

47	189	199	317
58	190	200	326
99	192	229	387
114	194	232	422
140	196	233	440

Low Temperature Specific Heat

17	146
26	179
42	305
56	312
64	379
69	404
112	

Magnetic Susceptibility

25	146	341
56	190	350
57	194	365
59	312	381
66	339	441

Neutron Scattering

21	53	82	165	194
26	61	83	177	203
30	65	84	185	327
38	66	87	186	351
41	79	89	189	367
43	80	119	190	396
51	81	122	191	

Nuclear Magnetic Resonance

22	99	205
25	110	314
26	120	401
42	153	415
58	159	454
61		

Optical Spectroscopy

23	114	188	210	396
24	115	189	211	401
60	140	191	215	404
68	141	192	219	407
71	143	194	220	413
74	156	200	228	415
90	157	201	386	426
113	187	209	395	

Positron Annihilation

41	90
78	161
86	

Sputtering

22	200
46	202
47	211
57	214
68	218
98	220
194	348

Synchrotron Radiation

24	92	203	392
58	113	230	394
66	170	347	421
84	175	389	455
85	196	391	456

Theory

Thermal Conductivity

Thermodynamics

X-Ray Photoelectron Spectroscopy

TECHNIQUE A22

X-Ray Scattering

24	76	172	203	376
25	84	175	211	389
26	85	186	216	391
30	86	188	217	392
38	87	189	218	400
41	107	192	220	414
42	119	196	305	415
43	122	200	315	419
57	134	201	347	421
66	160	202	351	453

Catalysis

32	71	150	226	398
36	77	152	228	400
39	92	171	324	420
58	111	194	368	421
62	120	199	370	445
66	121	200	386	452
68	144	203	391	

Channeling

88
389

Corrosion

12	103	154	218	328	389
52	106	178	222	331	394
67	135	200	232	354	405
70	136	204	233	372	425
71	137	206	234	375	426
73	147	214	325	380	429
96					

Crystal Structure, Atomic Distribution and Crystal Transformations

10	42	92	168	191	315
11	52	99	172	192	321
16	59	103	174	194	347
21	66	144	175	196	351
25	72	119	180	199	367
26	81	124	185	200	388
30	82	125	186	201	409
31	84	160	189	202	413
32	87	163	190	203	414
38	89	166			

Diffusion

3	76	164	214	333	406
4	86	178	215	337	412
7	101	185	216	344	419
12	105	186	218	348	422
41	110	187	223	352	424
43	118	188	225	353	428
46	128	189	231	365	435
47	135	192	318	371	440
61	149	194	321	372	450
67	151	198	327	401	454
72	161	200			

Dislocations

40	176	189	198	330	389
90	177	191	200	332	402
102	182	192	216	333	421
177	186	193	320	342	423
161	187	194	323	362	445
163	188	196	329	385	457

Erosion

50	182	232
68	200	233
96	214	317
137	224	354
173		

Electron and Ion Conduction

54	151	194	322	379	414
61	179	195	327	381	419
62	186	197	338	387	428
66	187	203	339	395	435
67	189	215	341	397	439
87	190	222	353	401	444
89	191	228	365	402	449
128	192	314	370	404	454
147					

Electronic Structure

Magnetism

Materials Preparation and Characterization

Nondestructive Evaluation

Phonons

Photovoltaic and Photothermal Phenomena

Point Defects

Precipitation

Recovery and Recrystallization

Sintering

Solidification

4	173	196	316
12	180	200	349
14	183	201	387
47	192	202	389

Strength/Fracture

6	94	193	335	405
7	95	195	346	406
8	102	212	352	429
9	106	213	360	430
11	125	222	366	432
20	155	224	376	438
48	173	231	378	443
50	176	304	383	450
79	177	319	399	451

Strength/
Constitutive Equations

40	336
163	374
306	431
334	442

Strength/
Fatigue

10	304	427
11	317	320
50	325	432
79	366	438
177	378	442
193	416	449

Strength/
Creep

40	177	306	364
50	193	332	365
79	216	336	416
106	304	356	431
136	305	361	436

Strength (continued)

Flow Stress

7	129	320	340	355
12	163	329	342	376
40	193	333	344	399
97	309	335	345	409
102	319	336	346	431
117	320			

Stress-Corrosion Cracking

8	213
31	222
73	375
149	389
206	429

Superconductivity

14	56	91	185	329
21	57	92	186	339
23	59	116	190	343
25	63	121	194	355
27	66	130	195	373
29	75	142	200	379
32	78	145	305	404
42	80	146	312	441
53	87	171	323	

Surface Phenomena and Thin Films

4	71	147	202	229	392
9	72	150	208	230	393
13	76	151	209	234	394
22	86	152	210	310	410
23	88	158	211	331	411
24	89	165	213	349	412
28	91	169	215	350	417
34	92	171	218	357	518
36	101	177	219	359	422
39	103	190	220	362	424
46	115	192	221	377	426
47	116	194	223	380	439
52	131	196	224	384	445
58	135	197	225	385	452
62	140	199	226	389	455
68	144	200	227	391	458

Welding

94	325
127	369
183	

Gas/Oxidizing

43	105	233	381
48	176	301	386
52	178	331	405
94	187	354	426
95	214	359	435
103	232	372	

Gas/
Hydrogen

7	76	149	223	366	400
18	88	164	224	368	406
21	92	166	231	375	411
31	101	194	304	380	414
41	110	198	315	392	420
48	121	201	333	393	424
59	133	211	350	398	427
68	138	213	354	399	451

Gas/
Sulphur-Containing

9	135	233	375
12	154	328	380
52	178	344	405
72	213	354	420
73	214	368	425
95	232	372	

Magnetic Field

23	66	190	329
33	134	195	339
58	185	303	357
59	186	312	441

Pressure Above Atmospheric

25	114	168	336
53	188	306	396
59	166	315	428
99			

Radiation/Electron

45	90	193	321
46	117	194	341
47	123	199	374
48	126	200	395
55	176	308	403
78	181	311	449

Radiation/Ion

45	161	197	308
46	176	199	311
47	181	200	337
48	190	215	341
55	192	216	403
78	194	217	407
160	196		

Radiation/Neutron

45	185	195	200
78	186	196	201
161	190	197	216
176	192	198	337
181	194		

Radiation/Photons

58	190	220
90	192	368
113	194	374
141	196	389
158	200	395
189	219	440

Radiation/Theory

46	181	374
47	194	457
90		

Radiation/Gamma

55	201	324
59	215	407
195		

Temperature

Very Low Temperatures

56	146	194	312
57	159	195	313
59	185	197	343
69	186	198	379
112	190	200	404
142			

High Temperatures

21	70	186	204	364	425
31	92	187	207	365	435
33	99	188	214	370	437
34	132	189	225	371	443
35	133	191	307	376	444
40	135	194	320	380	446
41	136	198	332	381	448
43	137	199	344	387	450
50	148	200	348	409	
52	168	201	353	423	
61	169	202	354		
67	185	203	363		

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