DOE/ER-0031

Materials Sciences Programs

FISCAL YEAR 1979

OFFICE OF BASIC ENERGY SCIENCES

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

September 1979

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UC-25

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FISCAL YEAR 1979

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U.S. Department of Energy
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Office of Energy Research
Washington, D.C. 20585

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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 D.O.E. 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, Nuclear Sciences, 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 1979 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 1979 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

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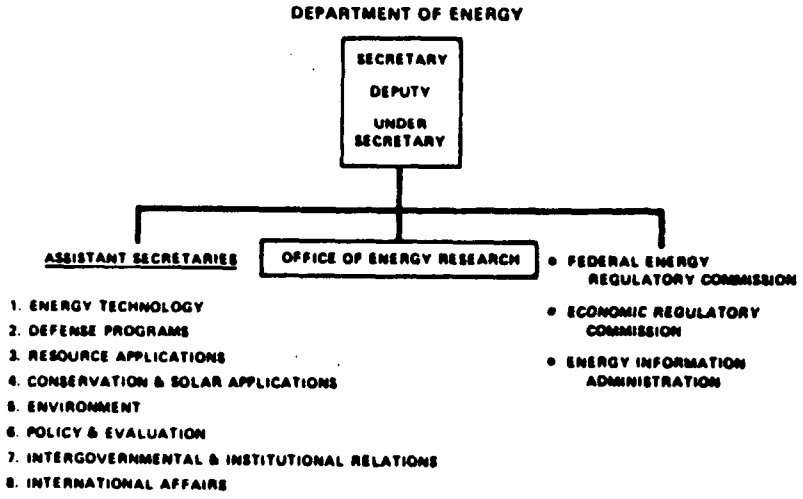

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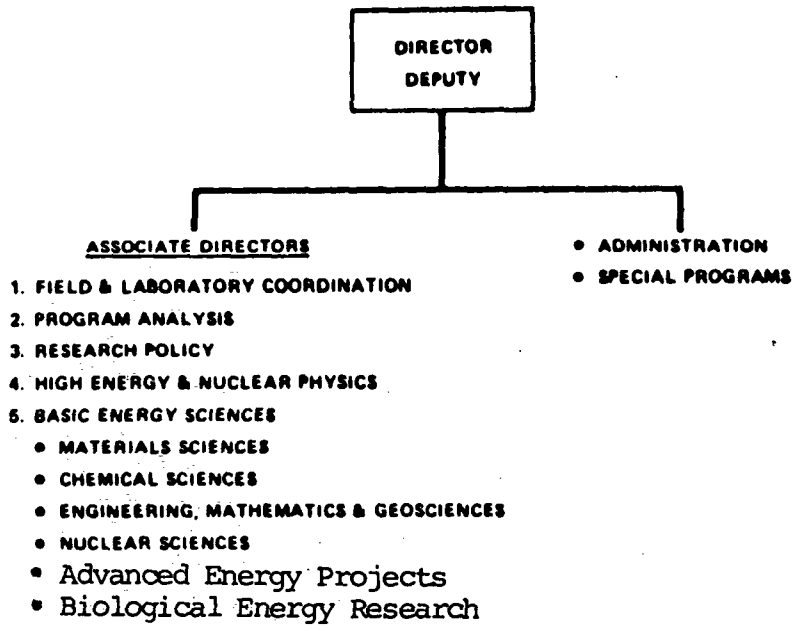

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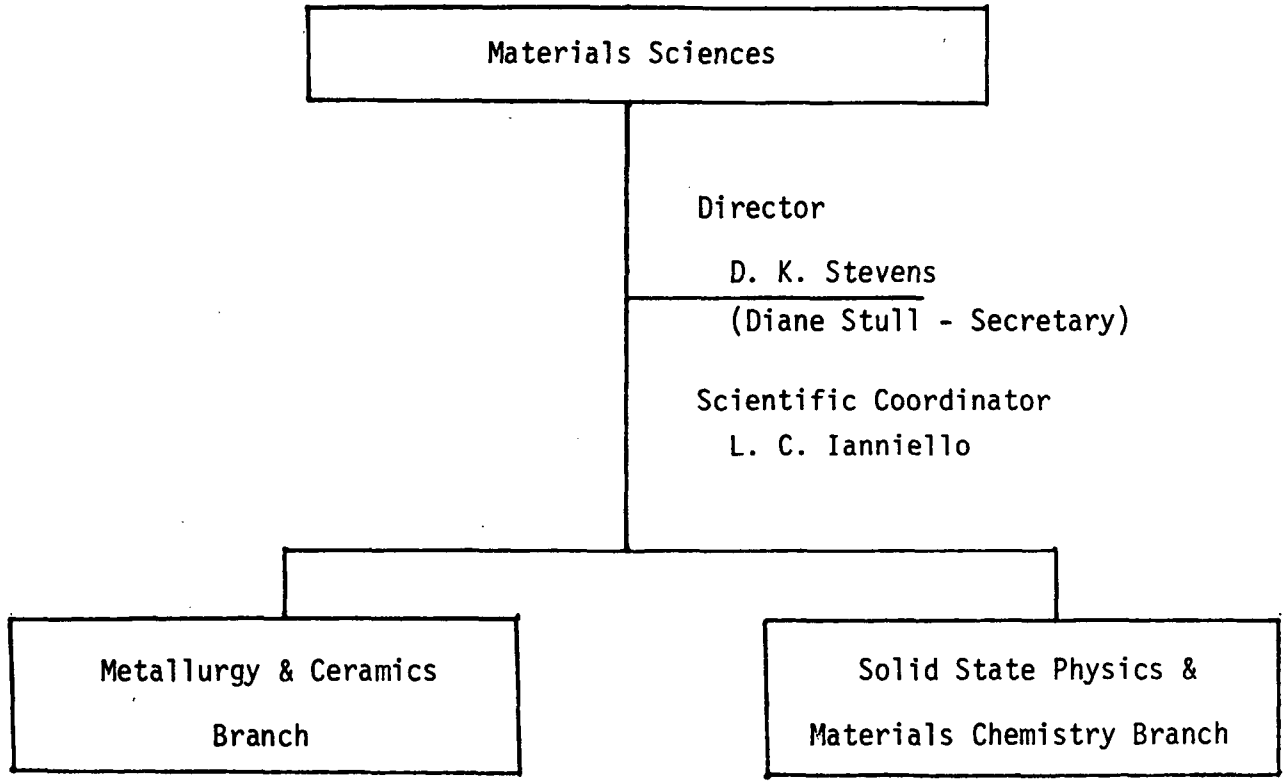

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F. V. Nolfi, Jr. 2/

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Notes: 1/ Returned to Ames Laboratory 8/79
2/ On Leave from ANL
3/ Returned to Georgetown University 8/79
4/ On Leave from LASL
5/ On Leave from Ames Laboratory

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SECTION A

Laboratories

The information was taken from current Laboratory program budget submissions. Most projects are of a continuing nature although specific problems and some projects were concluded in FY 1978.

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) 865-3930 or 515-294-3930

1. PHOTOVOLTAIC AND THERMOELECTRIC MATERIALS — $132,000 — 01-1
B. J. Beaudry, K. A. Gschneidner, Jr., F. A. Schmidt, R. K. Trivedi

Preparation of Schottky barrier solar cells by deposition of thin silicon films on refractory metal substrates (molybdenum and tantalum); in situ characterization of deposited films by Auger spectroscopy; use of SiO_2 and TaC to inhibit the formation of substrate silicides which may tend to prevent the attainment of large grain (>5 μm diameter) polycrystalline silicon. High temperature electric mobility and diffusivity measurements of silicon in tantalum. Development of procedures for preparing rare earth sulfides near the composition, $RS_{1.500}$ (candidate materials for photovoltaic conversion devices); low temperature heat capacity measurements and characterization studies of polycrystalline R_2S_3 phases.

2. THERMOTRANSPORT AND DIFFUSION STUDIES IN HIGH TEMPERATURE ALLOYS — $150,000 — 01-1
O. N. Carlson, F. A. Schmidt, R. K. Trivedi

Study of the migration of interstitial solutes in high strength, refractory metals subjected to large temperature gradients and the consequent degradation of the mechanical properties; thermotransport studies of carbon in vanadium, niobium and vanadium-titanium alloys. Electrotransport, thermotransport, and diffusion investigatons in iron-nickel alloys; application of these results to the interpretation of the thermotransport observations concerning carbon in vanadium and niobium alloys and to the development of a more general understanding of thermotransport phenomena.

3. PREPARATION AND CHARACTERIZATION OF HIGH PURITY MATERIALS — $108,000 — 01-1
B. J. Beaudry, O. N. Carlson, K. A. Gschneidner, Jr., F. A. Schmidt

Determination of the effects of nitrogen upon the deformation properties of vanadium over the temperature range 77-400 K; comparison of experimental results to theoretical predictions. Diffusion studies of iron in thorium; evaluation of the possibility that internal friction results constitute experimental evidence for the existence of a "diplon"

AMES LABORATORY
Metallurgy and Ceramics -01- (Continued)

interstitial, which has been postulated by others to occur in fast diffusing solute systems. Electrotransport purification of scandium, tantalum and niobium has produced ultra high purity samples for collaborative studies with numerous other investigators both in the U.S. and abroad. Electrotransport studies of carbon, nitrogen and oxygen in lanthanum and of iron, chromium, niobium, zirconium, and yttrium in lanthanum; diffusion coefficients, effective valences, and electric mobilities are evaluated. Preparation of high purity rare earths for local research programs, for collaborative work in domestic and foreign laboratories, and for use in special projects such as thermoelectric devices for space probes and materials for a highly successful adiabatic demagnetization refrigerator.

4. SOLIDIFICATION STUDIES — $ 48,000 — 01-1
R. K. Trivedi

Studies of dendritic growth in Ag-Pb, Ag-Bi and Pb-Sn systems will provide results with which an understanding of the solidification characteristics of the Cu-Nb system can be obtained; alloys of this system (Cu-Nb) are being used to prepare superconducting wire by controlled dendritic growth. Theoretical analysis of dendritic interfaces in binary alloys; the model predicts those morphological and parametric conditions which will exist in a binary system and which will control the microstructure of the cast alloys of that system.

5. ALLOY THEORY — $ 42,000 — 01-1
K. A. Gschneidner, Jr.

A new method for predicting the extent of terminal solid solubility which will exist in an alloy system was developed; the method is unique because it incorporates the proper effects of the electronic structures of the constituents upon the solubilities generated. This factor was not heretofore considered in solubility prediction schemes. The new method was shown to predict both extensive and limited solid solubilities with significantly higher reliabilities than other methods which do not employ the electronic structure factor.

6. MECHANICAL AND THERMAL PROPERTIES OF CERAMICS — $118,000 — 01-2
O. Hunter

Low temperature stabilization of tetragonal HfO_2. Significant amounts of the tetragonal phase were retained to room temperature through the thermodecomposition of $Hf(OH)_4$ and $HfOCl_2$ and the consequent production of the HfO_2 phase with an extremely small particle size; X-ray data indicate that the maximum particle size for the metastable phase produced by this method is approximately 100 Å. Stabilization of HfO_2 by hot pressing techniques; particles of metastable tetragonal HfO_2 as large as 500 Å were observed at room temperature. Thermocycling experiments of metastable HfO_2 were conducted to study the mechanical behavior as a function of amount of the metastable phase present.

AMES LABORATORY
Metallurgy and Ceramics -01- (Continued)

7. METAL HYDRIDES AND HYDROGEN IN METALS — $265,000 — 01-2
C. V. Owen, D. T. Peterson, T. E. Scott, S-a. Shei

Studies are being conducted of carbon doped vanadium, niobium and tantalum to determine the effect of carbon on the hydride formation temperature and hydrogen embrittlement. Hydrogen embrittlement characteristics of scandium and lutetium alloys (materials having an appreciable solubility for hydrogen) are being determined. Mechanical testing of hydrogen-charged, oriented single crystals of vanadium; effects of cold work on the hydrogen embrittlement behavior and upon the hydride formation temperature were studied by internal friction and Poynting effect measurements. The study of hydrogen attack on 1020 steel exposed to hydrogen at 900 and 1500 psi and 425°C for up to 16 days; the effects on yield stress and ultimate tensile stress were determined from tensile data; reduction in area, fracture stress, and density measurements were also made. Optical absorption measurements are being made on ScH_x, YH_x and LuH_x to provide information concerning the electronic structures of these compounds; excellent agreement is observed between these results (for low hydrogen concentrations) and band structure calculations made by other investigators. Thermotransport measurements for hydrogen and deuterium in vanadium, niobium, and tantalum.

8. TEMPER EMBRITTLEMENT AND STRESS CORROSION STUDIES — $ 58,000 — 01-2
C. V. Owen, S-a. Shei, T. E. Scott

The temper embrittlement phenomenon, observed in alloy steels, is being studied using Charpy tests and Auger-SIMS scans on a series of 3140 steel samples; results indicate a difference in the distribution of sulfur in the embrittled and deembrittled samples, which may be of significance to the understanding of the fundamental cause of the phenomenon. Stress corrosion studies are being initiated; microstrain experiments have been started on single crystals of high purity alpha brass.

9. ENVIRONMENTAL DEGRADATION OF MECHANICAL PROPERTIES — $ 63,000 — 01-2
K. Sieradzki

A new mechanical project has been initiated, which will involve the study of critical stress intensity factors of structural steels in agressive environments such as hydrogen or H_2S, CH_4, Cl_2 and I_2 atmospheres; a servohydraulic testing facility and environmental control chambers are being procured and placed into service.

AMES LABORATORY
Metallurgy and Ceramics -01- (Continued)

10. SHAPE MEMORY ALLOYS — $ 26,000 — 01-2
M. S. Wechsler

The unique ability to fabricate tubes of the Ni-Ti shape-memory alloy has been developed and the transformation properties of these samples are being evaluated by stress and strain measurements.

11. FABRICATION AND PHYSICAL PROPERTY STUDIES OF CERAMIC SYSTEMS — $135,000 — 01-3
M. F. Berard

Production, by the Ames toluene-acetone hydroxide precursor method, of HfO_2, Er_2O_3-stabilized HfO_2, and ThO_2 samples of near theoretical density. The method was also used, but with more limited success, in the preparation of ternary alloys of HfO_2-Er_2O_3-Ta_2O_5. Development of a method to suppress the ionic conductivity of Er_2O_3-stabilized HfO_2 through the alteration of the defect structure by using judicially selected pairs of stabilizing additives instead of a single stabilizing agent; Ta_2O_5 and Er_2O_3 are currently being evaluated. Study of the relative cation self-diffusion coefficients in the cubic and monolithic forms of Gd_2O_3. Study of the relationships between chemical stability and temperature for a glass used for the fixation of nuclear wastes.

12. BEHAVIOR AND PHYSICAL PROPERTIES OF SUPERALLOYS — $ 96,000 — 01-3
F. X. Kayser, J. D. Verhoeven

Investigation of the temperature dependence of the yield strength of Ni_3Al; elastic constants of oriented single crystals are being measured. X-ray diffraction, electrical resistance, and corrosion studies on a series of nickel-molybdenum alloys containing up to 20 at % Mo. Development of hot extrusion methods and techniques for iron-silicon alloys containing up to 25 at % Si. Production of superalloys by directional solidification techniques; study of the effects of composition, growth rate and temperature gradient upon convection in Nb-Al-Mo alloys.

13. PHYSICAL PROPERTIES OF REFRACTORY ALLOYS — $105,000 — 01-3
D. M. Bailey, J. F. Smith

Effects of interstitial elements upon properties of refractory metals; elastic behavior of interstitial solutions of the Th-C, V-O and Nb-H systems has been evaluated and work has been started on the Nb-Ta-H system.

AMES LABORATORY
Metallurgy and Ceramics -01- (Continued)

14. SUPERCONDUCTING MATERIALS AND SUPERCONDUCTIVITY — $198,000 — 01-3
D. M. Bailey, K. A. Gschneidner, O. D. McMasters, J. F. Smith, J. D. Verhoeven

Production of superconducting wire by controlled solidification; wire from Cu-Nb ingots is coated with tin and heat treated to form a highly effective superconducting material - resulting wire is equal or superior to commercially available superconducting wire. Thermodynamic data for Cu-Nb alloys are being determined from vapor pressure measurements via the Knudsen effusion method; results will be used to suggest appropriate alloying schemes to eliminate the undesirable monotectoid reaction caused in the Cu-Nb system by even relatively low levels of oxygen contamination. Superconductivity studies involving rare earth compounds; evaluaton of the possible superconducting characteristics of lanthanide compounds having lattice or structural instabilities which are analogous to instabilities observed in other known superconductors; La-Y-Mn alloys are presently being studied. The superconducting properties and T_c of Mo_2Be (which, according to calculations by E. S. Machlin-Columbia University, should have the highest T_c of any A15 type superconductor) are being evaluated; X-ray diffraction studies and microprobe analysis are being conducted to verify the stoichiometry of the compounds which have been produced.

15. ELECTRICAL AND MAGNETIC MATERIALS — $160,000 — 01-3
C. W. Chen, K. A. Gschneidner, Jr.

Heat capacity measurements as a function of magnetic field from 1-20 K on a high purity Tb single crystal; results will give the first experimental data regarding the magnetic field dependence of the heat capacity of a rare earth metal and should enable the evaluation of existing theories regarding the magnetic behavior of Tb. Development of high saturation amorphous iron alloys; splat cooled samples of the Fe-Ag-C system were found to have saturation values slightly higher than the best commercially obtainable material but still lower than the values desirable for use in high efficiency power transformers and other electrical machinery.

16. CONTROL OF MICROSTRUCTURES — $ 62,000 — 01-3
J. D. Verhoeven

The production of a dendritic morphology in Cu-Nb alloys (the morphology which is most desirable for the preparation of Nb_3Sn-Cu composite superconducting wire) can be achieved by the elimination of the eutectoid reaction caused by oxygen contamination; melting the Cu-Nb alloy in Y_2O_3 and ThO_2 crucibles results in oxygen concentrations below the

AMES LABORATORY
Metallurgy and Ceramics -01- (Continued)

level which produces the monotectoid reaction and the undesirable spheroidal morphology. Chill casting procedures which produce Cu-Nb ingots weighing up to 3 kilograms and having the proper microstructure for the production of superconducting wire; the casting technique development involved the optimization of atmosphere control, holding time and temperature, and pouring procedure.

17. PREPARATION AND PROPERTIES OF SINGLE CRYSTALS — $ 62,000 — 01-3
O. D. McMasters

Vertical zone melting, horizontal levitation zone melting, the Bridgman technique, and strain anneal methods are used to prepare single crystals of many rare earth metals and other materials. Some of those prepared this year for Ames Laboratory studies are: Ce, Pr, Nd, Gd, Zr, Ti, Hf, $CeSn_3$, and $LaSn_3$. In addition, the crystals are used by this group in a number of joint studies; those currently underway include: measurements of the thermoelectric power of Nd (with University of Birmingham); the study of magnetic exitations of Pr (with the Danish Atomic Energy Establishment, Risø, the University of Copenhagen, and Imperial College - London); diffusion studies of Au in Pr (with the Ben Gurion University - Israel).

18. LITHIUM ALLOYS FOR BATTERY APPLICATIONS — $ 32,000 — 01-3
D. M. Bailey, J. F. Smith

The lithium-tin system is being studied by thermal analysis, X-ray diffraction and metallographic techniques in order to provide complete and reliable crystallographic, thermodynamic, and phase relationship data for use in the development of lithium systems for battery and fusion applications.

19. RADIATION EFFECTS — $100,000 — 01-4
C. W. Chen, M. S. Wechsler

Helium bubble formation studies on V-Ti, V-Ti-Be, and V-Ti-Zr alloys; helium implantation or 4 MeV Ni^{++} irradiation was used to simulate radiation damage. The microstructural characteristics which should be most successful in the obviation of the effects of helium bubble formation in the first wall of a fusion reactor were deduced. A theoretical analysis was conducted of the trapping of interstitial impurity atoms at irradiation produced defect clusters; good agreement with the observed experimental results for oxygen trapping in vanadium was observed.

AMES LABORATORY
Metallurgy and Ceramics -01- (Continued)

20. NONDESTRUCTIVE EVALUATION $150,000 01-5
C. P. Burger, K. G. McConnell,
L. W. Schmerr, L. W. Zachary

Development of the boundary integral equation (BIE) method for predicting the ultrasonic scattering of two dimensional flaws in solids; the results provided by a first generation program for the BIE method have been compared with the known solution for ultrasonic scattering from a cylindrical void - excellent agreement was observed. Work has been initiated on the development and testing of the singularity expansion method (SEM) for extracting the complex resonances of a system from its transient response; when fully developed, the method promises to provide an effective procedure for obtaining information for the characterization of flaws in solid materials. The use of dynamic photoelasticity for the characterization of ultrasonic wave interactions with surface breaking cracks; a photoelastic material (CR39 by Homolite) was chosen and a high-speed, dynamic photographic technique utilizing a Cranz-Schardin spark camera was adopted.

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

21. NEUTRON SCATTERING $260,000 02-1
W. A. Kamitakahara, D. Khatamian,
G. R. Kline, C. Stassis

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); electronic structure of mixed valence compounds ($CeSn_3$, Ce_xTh_{1-x}); study of the effect of hydrogen and carbon impurities on the properties of metals (Th-H, Y-H, La-H).

22. SEMICONDUCTOR PHYSICS $167,000 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 and SIMS studies of surfaces and interfaces: 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 Division -02- (Continued)

23. NUCLEAR RESONANCE IN SOLIDS $146,000 02-2
R. G. Barnes, D. R. Torgeson

Applications of nuclear magnetic resonance, nuclear quadrupole resonance, and Mossbauer effect to: determination of hydrogen-isotope locations and diffusion parameters in hydride and deuteride phases of refractory metals (e.g., V, Nb, Ta), alloys (e.g., Nb-Ti, Nb-V), and compounds (e.g., Ta_6W, V_2C); electronic and structural phase transitions in refractory metal hydrides; interactions between hydrogen isotopes and interstitial impurities such as O, N, and C in refractory metals (V, Nb, Ta); electronic structure, charge density wave effects, and structural transformations in one and two-dimensional metallic compounds (e.g., ScCl, $CsScCl_3$, $BaVS_3$).

24. SUPERCONDUCTIVITY $317,000 02-2
D. K. Finnemore, T. Y. Hsiang,
J. W. Osmun, J. R. Ostenson,
E. L. Wolf, R. J. Noer

Investigations of strong-coupling transition metal, transition metal alloy, and transition-metal compound superconductors using proximity electron tunneling spectroscopy (PETS), electron energy loss spectroscopy (ELS), Auger analysis and ultraviolet photoemission spectroscopy (UPS). Development of superconducting composites suitable for large scale magnets in the 8 to 14 Tesla range; fundamental studies of superconductivity in inhomogeneous materials; practical studies to improve wire fabrication techniques, and performance characteristics such as critical currents, and ac losses.

25. OPTICAL AND SPECTROSCOPIC PROPERTIES OF SOLIDS AND LIQUIDS $346,000 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): transition metal alloys and compounds (e.g., FeTi), transition metal-hydrogen systems, A15 superconductors (Nb_3Ge); GaAs, layered transition metal chalcogenides (MoS_2); amorphous metals. Photoemission into liquid electrolytes, electrochemical modulation spectroscopy, surface Raman scattering, and photoelectrochemistry: 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.

AMES LABORATORY
Solid State Physics Division -02- (Continued)

26. MATERIALS FOR HYDROGEN STORAGE $135,000 02-2
R. G. Barnes, J. D. Corbett,
K. A. Gschneidner, Jr., D. T. Peterson,
C. J. Stassis

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.

27. MAGNETIC PROPERTIES OF SOLIDS $60,000 02-2
S. Legvold

Experimental magnetic and transport properties of rare earth alloys; search for Lifshitz critical points (Gd-Lu, Tb-La); magnetic critical temperature gap (Gd-Y); crystal field effects in light-heavy rare earth single crystals (Dy-Pr, Tb-Pr); magnetoresistance of Gd-Y alloys.

28. NEW MATERIALS $184,000 02-2
R. N. Shelton, C. A. Swenson,
M. S. Anderson

Synthesis of new ternary compounds (e.g., $LaPt_2Si_2$) 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.

29. MAGNETIC AND ELECTRONIC PROPERTIES $155,000 02-3
B. N. Harmon, K. M. Ho,
R. A. Klemm, S. H. Liu

Electronic properties of transition and rare-earth metals and compounds (ZrB_2, ZrS, ScS, PtTe, YH_2, ScH_2). Theory of soft modes and lattice instabilities in metals and metallic compounds and their relation to the electron-phonon interaction and superconductivity (Nb, Zr, Ti, Mo). Electronic and magnetic properties of mixed valence compounds ($CeSn_3$). Static and dynamic properties of spin glasses. Electronic structure of the surface of metal electrodes (e.g., Ag); microscopic properties of the metal-electrolyte interface.

AMES LABORATORY
Solid State Physics Division -02- (Continued)

30. OPTICAL AND SURFACE PHYSICS THEORY $151,000 02-3
R. Fuchs, K. L. Kliewer,
J. Reyes

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 with emphasis on surface states. Photoemission into liquid electrolytes and related catalytic, electrochemical, adsorption, and corrosion effects; anodic photocurrents; the liquid metal interface. Solar energy studies: electrochemical photovoltaic cells, photolysis, high-temperature adsorbers, and optical properties of phase-change materials for solar applications.

31. SUPERCONDUCTIVITY THEORY $ 94,000 02-3
J. R. Clem, R. A. Klemm,
K. Machida, 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

32. X-RAY AND NEUTRON CRYSTALLOGRAPHY $183,000 03-1
R. A. Jacobson, B. J. Helland,
M. Gress

Development of diffraction techniques and service facilities; indirect methods and refinement techniques; structural studies of intercalated transition metal dichalcogenides; metal complex structures with emphasis on model homogeneous catalysts and polymetal species; intramolecular solid state interactions which modify properties of parent species; radial distribution function analysis of coal's amorphous scattering.

AMES LABORATORY
Materials Chemistry Division -03- (Continued)

33. METAL-METAL BONDING IN SOLID STATE MATERIALS — $170,000 — 03-1
J. D. Corbett, R. C. Burns

Synthesis and characterization of new types of reduced inorganic compounds at high temperature (e.g., of Sc, Ti, Zr, Nb, Mo, rare earths); extended metal-metal bonding; catalytic activity and hydrogen storage potential of new types of reduced compounds; stress-corrosion-cracking by zirconium iodides in nuclear reactors; homopolyatomic ions (e.g., of Ge, Sn, Sb, Bi, Te); ionic intermetallic phases.

34. CHEMISTRY OF HEAVY TRANSITION METALS — $147,000 — 03-1
R. E. McCarley

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

35. METALS FROM FLY ASH — $120,000 — 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.

36. HIGH TEMPERATURE BEHAVIOR OF METALS — $ 82,000 — 03-2
R. G. Bautista

Correlation and prediction of heat capacity, heat content, and heat of mixing of liquid Cu-Ce alloys by levitation calorimetry; normal spectral emittance of liquid iron, nickel, and Cu-Ce alloys using a blackbody comparison method; practical temperature measurements of liquid metals and alloys by optical pyrometry; corrosion of high chromium alloys by O_2 and SO_2, including scale resistance and chemical reactions; re-evaluation of available experimental data using Bartlett's model to predict the oxidation state of alloys.

AMES LABORATORY
Materials Chemistry Division -03- (Continued)

37. PARTICULATE PROCESSING $118,000 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 operations involving the preparation of ceramic powders (yttria and urania); reaction kinetics and mixing in multicomponent mass transfer systems involving chemical reactions with emphasis on correlation between theory and experiment (nuclear fuel reprocessing and metal recovery processes).

38. HIGH TEMPERATURE CHEMISTRY $180,000 03-3
H. F. Franzen, R. A. Schiffman,
J. Anderegg

Structure and bonding in refractory and corrosion-resistant compounds, particularly metal-rich transition metal chalcogenides (ZrS, ScS); phosphides (e.g., Sc, Ti, Va) and nickel aluminide; stability, phase equilibria, X-ray diffraction, photoelectron spectroscopy, and mass spectrometry studies of Y, La and Sc phosphides at high temperatures; band structure and electronic properties of ZrS and ScS.

39. SURFACE CHEMISTRY AND CATALYSIS $293,000 03-3
R. S. Hansen, B. Parkinson,
K. G. Baikerikar

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; 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., $MoSe_2$, WSa_2, GaS_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

40. ALLOY PROPERTIES $518,000 01-1
D. J. Lam, A. T. Aldred,
A. J. Arko, G. S. Knapp,
B. W. Veal, D. P. Karim,
P. Georgopoulos

Studies of electronic structure and its relationship to physical properties and bonding; emphasis on actinide metals, alloys and compounds; studies of bonding of metal oxides (transition metals, rare-earths and actinides) in silicate based glasses by means of x-ray photoemission spectroscopy (XPS), extended x-ray absorption fine structure (EXAFS) and magnetization measurements; alloy chemistry studies of actinide compounds and actinide-alkali-silicate glasses; studies of Fermi surface in actinide metals and intermetallic compounds via deHaas van Alphen effect; experimental and theoretical studies of the electronic structure of hydrogen in metals and amorphous silicon.

41. SCATTERING STUDIES $613,000 01-1
M. H. Mueller, G. H. Lander,
J. E. Epperson

Magnetic, electronic and structural properties of actinide materials using neutron and x-ray scattering; particular emphasis on measurements on single crystals using both elastic and inelastic neutron scattering techniques; structural investigations of Pd and Nb hydrides and deuterides, and studies of storage metal hydrides of the type $LaNi_5H_6$; programs at the ANL pulsed neutron source involving both structural and dynamical studies; e.g., application of high-resolution powder techniques to various materials including complex hydrides, inelastic neutron experiments on UO_2; x-ray diffuse scattering of metallic and ceramic-type materials.

42. CATALYSIS AND SURFACE STUDIES $241,000 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; low energy electron diffraction; x-ray and ultraviolet photoelectron spectroscopy; electron loss spectroscopy; Auger electron spectroscopy; thermal desorption; and surface vibrations.

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

43. CONSTITUTIVE RELATIONS $190,000 01-2
A. P. L. Turner, U. F. Kocks,
J. L. Routbort

Formulation of equation-of-state-based constitutive laws to describe the deformation behavior of metals and ceramics particularly at high temperature where time-dependent processes are important; application of these laws to the prediction of material behavior during complex loading histories, and to modeling of material forming processes.

44. STRENGTH AND DEFORMATION OF MATERIALS $228,000 01-2
A. P. L. Turner, U. F. Kocks,
J. L. Routbort, R. O. Scattergood,
R. B. Schwarz

Investigation of the nature of plastic deformation of metals and ceramics; theoretical and experimental studies of the mechanisms of strengthening including precipitation, solution and deformation hardening, and dynamic strain aging; formulation of unifying constitutive laws based on an understanding of the underlying mechanisms of strengthing and deformation applicable over the widest possible range of temperature, strain rate and stress; studies of material behavior during transient and cyclic conditions; techniques employed include mechanical testing, in-situ HVEM experiments, TEM, computer modeling, and internal friction.

45. METAL PHYSICS $919,000 01-3
R. W. Siegel, A. S. Berger
E. S. Fisher, M. J. Fluss,
N. Q. Lam, J. N. Mundy,
S. J. Rothman, L. C. Smedskjaer,
D. J. Westlake, B. Chakraborty

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 surfaces and interfaces; hydrogen solubility limits and the properties of metal-hydrogen systems; studies of metals, including bcc refractory metals, alloys and intermetallic compounds using position annihilation spectroscopy, tracer diffusion, resistometry, transmission-electron and field-ion microscopy, neutron and x-ray diffraction, and ultrasonic-wave propagation.

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

46. SUPERCONDUCTIVITIY $236,000 01-3
A. T. Aldred, A. J. Arko
F. Y. Fradin, G. S. Knapp,
P. Georgopoulos, P. K. Tse

Studies of the effects of structural defects, lattice transformations, and localized magnetic moments on the electron-phonon interactions and superconducting proeprties of ternary molybdemum chalcogenides and ternary rhodium borides by nuclear magnetic resonance, magnetization, heat capacity, and Mössbauer effect measurements, EXAFS and heat capacity studies of anharmonic behavior on the superconducting properties of A-15 compounds; de Haas van Alphen effect in A-15 compounds.

47. BASIC CERAMICS STUDIES $590,000 01-3
N. L. Peterson, W. K. Chen,
J. Faber, Jr., M. D. Rechtin,
D. Wolf, R. J. Friauf,
K. Y. Liou

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, and Mössbauer techniques; ionic transport mechanisms in sodium beta-alumina; defect-solute interactions and defect clustering in oxides; theoretical studies of kinetic processes in 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; oxidation processes in nonstoichiometric oxides using the environmental cell in the HVEM; radiation damage in ceramics and glasses; preparation of single crystals of metal oxides.

48. NEUTRON IRRADIATION STUDIES $726,000 01-4
T. H. Blewitt, R. C. Birtcher,
B. S. Brown, M. A. Kirk, Jr.,
B. A. Loomis

Design 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.

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

49. CHARGED PARTICLE IRRADIATION STUDIES — $440,000 — 01-4
K. L. Merkle, R. S. Averback,
R. Benedek, W. E. King

Damage function studies in metals by ion irradiation, HVEM and field ion microscopy; defect production at elevated temperature; structure of cascades by TEM, HVEM, and computer simulations. Interaction of cascade structures with point defects by ion irradiation and HVEM; energy density effects in cascades by molecular ion bombardment; diffusion and trapping of implanted hydrogen and helium in metals; interatomic potential calculations; defect and ion-solid interaction studies by ion scattering techniques; effect of crystallinity of defect production; formation and properties of radiation induced defect clusters. Major experimental facilities; 300keV heavy ion accelerator.

50. KINETICS STUDIES — $715,000 — 01-4
H. Wiedersich, F. V. Nolfi, Jr.,
P. R. Okamoto, D. I. Potter,
P. P. Pronko, A. Taylor,
L. E. Rehn

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; irradiation creep; radiation sources include 4 MV Dynamitron-2 MV Van de Graaff dual-ion-beam facility.

51. HIGH VOLTAGE ELECTRON MICROSCOPE TANDEM FACILITY — $226,000 — 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, and specific gaseous environments are in use; the interface to 300 kV ion accelerator will be completed in FY 1979; 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.

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

52. MECHANISMS OF FAILURE OF MATERIALS $198,000 01-5
A. P. L. Turner, R. A. Mulford,
J. L. Routbort, R. O. Scattergood

Investigations of critical processes that lead to component failures including creep fracture, fatigue, erosion and erosion corrosion; emphasis is on understanding microscopic mechanisms such as grain boundary cavitation, impurity segregation to grain boundaries, crack-tip-zone processes, and microcrack formation. The role of microstructural inhomogeneities and external environments including radiation are studied. Test materials are both metals and ceramics.

53. NONDESTRUCTIVE EVALUATION $255,000 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').

54. CORROSION STUDIES $230,000 01-5
M. B. Brodsky, R. L. Lyles, Jr.,
L. E. Rehn, J. R. Chen

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, kinetic studies and ion-bean analysis; alloy modification by ion beam implantation for corrosion studies; effects of stress on oxidation and sulfidation; Ni-Cr; Ni-Al; Fe-Cr; and Fe-Al alloys.

ARGONNE NATIONAL LABORATORY
Intense Pulsed Neutron Source Program -02
D. L. Price, Phone (FTS) 972-5518 or 312-972-5518

55. PULSED NEUTRON SOURCE DEVELOPMENT 02-1
D. L. Price, J. M. Carpenter, R. L. Kustom, N. J. Swanson, J. H. Talboy

The IPNS Program has the goal of providing an intense 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 Upgrade construction project, for which $ 3.0 M has been requested beginning in FY 1980, to complete the initial reseach 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 on which scientific data will be obtained and experience in targetry and instrumentation will be derived; the operating phase will proceed 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
9700 South Cass Avenue
Argonne, Illinois 60439

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

56. NEUTRON SCATTERING RESEARCH — $1,718,000 — 02-1
T. O. Brun, G. Felcher, J. Jorgensen, T. Kajitani, C. Pelizzari, T. Postol, J. Rotella, S. Sinha, K. Sköld, P. Vora

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, ferroelectrics, dynamics of hydrogen in solid and liquid metals, and molecules adsorbed on surfaces. Steady-state and time-of-flight techniques are employed at the CP-5 reseach reactor, while increasing use is being made of the prototype pulsed source based on proton spallation reactions. A major effort is devoted to development of instrumentation for use with pulsed neutron sources such as IPNS. Facilities include a thermal neutron time-of-flight spectrometer, triple-axis spectrometer, time-of-flight diffractometer, a two-axis diffractometer, as well as high-pressure and high-magnetic-field facilities. Current areas of interest include the structure and lattice dynamics of hydrides; the dynamics of amorphous As and liquids including He^3 and Ar^{36}; melting of crystalline solids; the structure of dense molecular gases including N_2O_2, CO_2 and C_2H_2; phase transitions in ferromagnetics; dynamics of superconductors and solid electrolytes; crystal-field interactions and magnetic properties of transition metals and alloys and of rare-earth intermetallics; magnetic scattering in magnetically ordered systems and spin glasses; high-pressure diffraction and compressibility measurements of metals, ionic crystals, ice and high-temperature ceramics.

57. MATERIALS PREPARATION AND CHARACTERIZATION — $181,000 — 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; refractory oxides; Chevrel-phase compounds; ternary borides; orthohombic NaCN; and transition metal beryllides.

ARGONNE NATIONAL LABORATORY
Solid State Science Division -02- (continued

58. OPTICAL, TRANSPORT AND RADIATION PROPERTIES OF INSULATORS — $613,000 — 02-2
C. J. Delbecq, J. J. Jackson, S. A. Marshall, W. Primak and P. H. Yuster

Study of defects in nonmetallic crystals caused by added impurities or by exposure to ionizing radiation. Major areas of activity include: Tunneling recombination luminescence between trapped electrons and trapped holes in both alkali halide crystals (KCl:AgCl) and refractory oxide crystals (Al_2O_3:Cr_2O_3); thermally activated formation of electrons or holes in refractory oxides containing transition metal ion impurities (Al_2O_3:Co_2O_3:V_2O_3); production and motion of interstitials in alkali halides (FCl^- in KCl and KF); the use of paramagnetic ions as probes to study defect production in refractory oxides (Y_2O_3:Gd_2O_3); the study of defect formation by the production of nonstoichiometry upon exposing Y_2O_3 at high temperatures to oxidizing and reducing atmospheres; 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.

59. VERY LOW TEMPERATURE STUDIES — $191,000 — 02-2
P. Roach, L. Jedrzejek

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; development of SQUID NMR technqiues for susceptibility measurements in the low millikelvin range; static and dynamic susceptibility of He^3 phases; and the search for triplet or p-wave superconductviity in metals.

60. TUNNELING AND TRANSPORT PROPERTIES — $300,000 — 02-2
C. Falco, K. Gray, R. Kampwirth, T. Lee, I. Schuller, H. Willemsen

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 nonequilibrium 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; modulated films; transport properties measurement; study of relaxation times in a magnetic field. The following applications have resulted from these studies: fault current limiter; high temperature SQUID development; superconducting transistor; superconducting filters; geophysical propspecting using SQUIDS.

ARGONNE NATIONAL LABORATORY
Solid State Science Division -02- (continued)

61. STUDIES OF CATALYSTS AND SURFACES — $223,000 — 02-2
B. Abraham, L. Iton, K. Miyano, D. O'Reilly

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 dactive solutes.

62. ELECTRONIC, MAGNETIC AND LATTICE PROPERTIES — $409,000 — 02-2
G. Crabtree, B. Dunlap, W. Johanson, H. Kierstead, D. Niarchos, G. Shenoy, J. Viccaro

Mössbauer effect studies of ternary superconductors such as $(Sn,Eu)Mo_6S_8$, $ErRh_4B_4$ and related materials; crystal field and magnetic ordering in rare earth hydroxides; 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, measurement 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, UIr_3); mixed valence and other rare earth materials (Lu, $LaSn_3$, $CeSn_3$); superconducting A-15 compounds (Nb_3Sb).

ARGONNE NATIONAL LABORATORY
Solid State Science Division -02- (continued)

63. OPTICAL AND ELECTRONIC PROPERTIES OF SEMICONDUCTORS — $259,000 — 02-2
L. Guttman, R. Kampwirth, J. McMillan, 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 porperties of chemically modified amorphous sytems.; studies of the random network model of amorphous materials; and theoretical limits on attainable optical properties.

64. SOLID STATE THEORY AND COMPUTER SIMULATION — $489,000 — 02-3
T. Arai, T. Gilbert, C. Hsu, D. Koelling, A. Rahman, J. Robinson, 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.

65. GEOTHERMAL PROSPECTING WITH SQUIDS — $99,000 — 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).

66. 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 1980.

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

67. CHEMICAL STRUCTURE: NEUTRON SCATTERING, X-RAY AND EXAFS STRUCTURAL STUDIES — $722,000 — 03-1
S. W. Peterson, M. Atoji, J. M. Williams, A. H. Reis, Jr., A. J. Schultz, E. G. Sherry, R. K. Brown, T. Morrison

The major goals are the study and development 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. Current emphasis is on inorganic one-dimensional (1-D) Pt-chain conductors, organic 1-D conductors related to tetracyanoquinodimethane (TCNQ), tungsten bronzes, hydrogenation and methanation catalysts, magnetic-moment structural studies of rare-earth metals, alloys and compounds, expanded structural studies of the catalytic activation of C-H bonds, and studies of metal-exchanged zeolite systems. A major effort in support of IPNS is the design and construction of a time-of-flight, pulsed-beam, neutron diffractometer for single-crystal studies. A polarized neutron instrument is also under development in collaboration with ANL's Solid State Science Division.

68. HIGH-TEMPERATURE MATERIALS CHEMISTRY — $469,000 — 03-3
R. J. Thorn, G. L. Bullard, K. D. Carlson, G. E. Murch, E. G. Rauh, G. H. Winslow, J. Ziomek

The program emphasis is on investigations of the fundamental concepts in high-temperature solid-state chemistry in terms of point defects, altered valent cations, electronic structures, phonon-electron interactions, and studies of chemical bonding in ionic crystals and in ionic-covalent and metallic ceramic materials. Interionic potentials are used in Monte Carlo calculations and computer simulations to derive thermodynamic and transport data. Investigations are made of reactions associated with diffusion limited sublimation, creep and sintering, and nonequilibrium condensation of high-temperature vapors to amorphorus materials with metastable valence states. Quantitative electronic structures are determined from x-ray photoelectron spectroscopic measurements. Partial molar thermodynamic properties and diffusion in nonstoichiometric phases are measured and equations of state and transport for computer codes of performance of nuclear, MHD, and CTR materials are derived. Oxides and carbides of actinide and rare-earth elements, glasses for waste storage, electronic conducting ceramics, electrode materials and insulators are the materials currently being studied.

ARGONNE NATIONAL LABORATORY
Chemistry Division -03- (continued)

69. PHYSICAL AND SURFACE CHEMISTRY OF ENERGY SYSTEMS — $462,000 — 03-3
D. M. Gruen, A. R. Krauss, M. H. Mendelsohn, M. J. Pellin, C. O. Steinbruchel, A. F. Wagner, R. B. Wright

Laser fluorescence spectroscopy of sputtered atoms, ions and molecules are studied to determine internal state, energy and angular distributions, sputtering yields and ion fractions. This work coupled with studies of secondary-photon emission, energy-analyzed secondary-ion mass spectrometry, and simultaneous in situ Auger and XPS determinations of fractional monolayer coverages of active gases allows one to obtain ionization coefficients at surfaces. Models of charge transfer processes and excitation and de-excitation mechanism at surfaces are being elaborated and tested against experimental results. Several surface analytical techniques (energy-analyzed SIMS, SCANIIR, Auger, XPS, SEM, MIS, TED, glancing-angle x-ray diffraction, laser Raman scattering) are being used to elucidate the effects of surface chemistry in modifying the total interaction process of energetic reactive particles with target surfaces. Properties of group III A and group IV A element substituted AB_5 hydrides are studied, and the relationship between thermodynamic stability and structure is being determined. Cryochemistry and photochemistry of matrix-isolated metal atoms, clusters and molecules are studied to develop a better understanding of catalysts and of catalytic mechanisms.

70. CALORIMETRY AND THERMODYNAMICS — $170,000 — 03-3
P. A. G. O'Hare, H. E. Flotow, D. Ohlendorf

Heat capacity, entropy, enthalpy increments, enthalpies of formation, and free energies of formation are measured, calculated and evaluated. Thermal 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 measure the heat capacity of well-characterized materials from liquid helium temperatures to 350 K. Recent emphasis has been on metal hydrides, Pu_2O_3, Cr_3CrO_4, rare-earth fluorides, and $LaCrO_3$.

ARGONNE NATIONAL LABORATORY
Chemical Engineering Division -03-
L. Burris - Phone: (FTS) 972-4314 or 312/972-4314
F. Cafasso - Phone: (FTS) 972-4542 or 312/972-4542

71. LIQUID METAL CHEMISTRY $265,000 03-2
V. A. Maroni, E. Veleckis,
W. Calaway, R. Yonco

Thermodynamic properties of liquid metals and intermetallic compounds with emphasis on alkali-metal based systems; temperature, composition and pressure relationships in selected ternary hydrides (e.g., LiAlH, CaAlH, LiPbH) systems, solubilities and interaction chemistries of nonmetals in liquid metals; distribution of nonmetals (e.g., nitrogen and carbon) in lithium/molten salt and lithium/structural material systems; corrosion mechanisms of refractory metals and alloys in liquid metals.

72. CHEMISTRY OF MATERIALS $385,000 03-2
R. Kumar, B. Holt
B. Hubble, S. Siegel
S. Johnson

Chemistry of airborne particulates; elucidation of formation mechanisms for sulfates, nitrates and organics; development of instrumentation for sampling and real time characterization of aerosols. Investigation of the hydrolysis-oxidation conversion of sulfur dioxide to sulfate by stable isotope ratio measurements; study of the influence of pH, oxides of nitrogen, and of reactive surfaces (e.g., airborne carbonaceous materials) on this conversion; kinetics and mechanisms of mineral-sulfur dioxide reactions and mineral regeneration reactions; study of structure and morphology accompanying reaction sequence; development of reaction models and prediction capability.

73. PHYSICAL CHEMISTRY OF ELECTRO-CHEMICAL SYSTEMS $180,000 03-2
Z. Nagy, C. Melendres
M. Blander, M.-L. Saboungi

Kinetics and mechanisms of processes occurring at cell electrodes and in electrolytes; study of metal (Fe, Ni, Cu) and sulfide (FeS, NiS) dissolution/deposition reactions in molten electrolytes by relaxation and rotating-disc electrode techniques; thermodynamic measurements on alloys emphasizing systems that show promise as battery electrodes (e.g., LiPb); prediction of thermodynamic properties of ternary alloys and their phase diagrams using fundamental solution theories.

ARGONNE NATIONAL LABORATORY
Chemical Engineering Division -03- (continued)

74. CALORIMETRIC STUDIES OF ENERGY RELATED MATERIALS — $145,000 — 03-2
P. A. G. O'Hare, C. E. Johnson
W. N. Hubbard, G. K. Johnson

Measurement of thermochemical properties of organic and inorganic materials; prediction of enthalpies of formation, bond energies and molecular stabilities; enthalpies of formation of (1) heteroatomic polyaromatic molecules (e.g., benzonapthofuran, chromone, thioxanthone, etc.) that are "building block molecules" of coal, and (2) enthalpies of formation and hydrogenation of AB_5-rare earth-transition metal alloys (e.g., $LaNi_5$) and related compounds with aluminum (e.g., $LaAlNi_4$) that are potential hydrogen-storage systems. Emphasis is on developing relationships between heats of formation (and/or hydrogenation) and bond type, or structure, or both for predictive purposes; critical compilations of thermodynamic data; measurement techniques include oxygen, fluorine, and hydrogen-bomb calorimetry, hypergolic and flow calorimetry, and drop calorimetry to 2000°C.

75. CHEMISTRY OF MOLTEN SALTS AND METALLURGICAL PROCESSES — $230,000 — 03-2
M. Blander, Z. Nagy
M.-L. Saboungi, J. Settle

Derivation of theories of high temperature multicomponent solutions; prediction of thermodynamic properties and phase diagrams of molten salts using fundamental solution theories; application of theories to slags and to solutions containing acid salts ; measurement of the solubilities of metal sulfides (e.g., FeS, PbS) in molten salts; study of sulfide-polysulfide equilibria and complexing of cations by anionic species in molten salts. Research on fundamental chemistry of electrowinning of metals; impurity interaction studies in chloride melts; electro-dissolution of sulfide ores.

76. SURFACE, STRUCTURAL, AND MORPHOLOGICAL STUDIES ON ELECTROCHEMICAL SYSTEMS — $190,000 — 03-2
S. Siegel, C. Melendres
F. A. Cafasso

Surface, structural, morphological and theoretical studies of electrode processes; *in situ* investigations of electrocatalysis mechanisms and electrode corrosion phenomena using coupled spectroscopic (visible, Raman/Mossbauer) and electrochemical techniques; study of oxygen reduction at organo-metallic electrode (e.g., iron pthalocyanine and phorpyrins on carbon) systems; research on investigation of the kinetics and mechanisms of anodic corrosion and passivation of metals (e.g., Fe, Pb, Co) in aqueous and molten salt electrolytes; X-ray diffraction structural studies of Li-Fe-S phases formed during charging of LiAl/FeS cells.

ARGONNE NATIONAL LABORATORY
Chemical Engineering Division -03- (continued)

77. HEAT TRANSFER MATERIALS AND SALT VAPORS — $130,000 — 03-2
L. Curtiss, D. Frurip
M. Blander

Experimental and quantum mechanical studies on materials that exhibit molecular associations in the vapor and that may either have potential as heat-transfer fluids or can enhance gas phase mass transport; emphasis is on the nature of the species, their structure, bond strengths and association constants; systems under investigation include acetic acid, trifluoracetic acid, binary mixtures of these compounds with water as well as complexes formed between selected metals (e.g., beryllium and magnesium) and water; thermal conductivities and vapor densities of high temperature associated systems; statistical mechanical prediction of the thermodynamic properties of high temperature ionic molecules.

78. SPECTROSCOPY OF SEPARATION PROCESSES — $75,000 — 03-2
G. Papatheodorou

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/actinide metal 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.

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

79. INTERGRANULAR STRESS CORROSION — $200,000 — 01-2
J. R. Weeks, Brijesh Vyas,
M. W. Kendig, H. S. Isaacs,
C. S. Pande

Electrochemistry of surfaces of iron and nickel base alloys at high temperatures using an ac polarization technique. Development of a 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.

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

80. BASIC PROCESSES AND MICROSTRUCTURAL PROPERTIES OF AMORPHOUS SEMICONDUCTORS — $150,000 — 01-1
R. W. Griffith, F. J. Kampas,
P. E. Vanier, M. D. Hirsch

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.

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

81. RELATIONSHIP BETWEEN PROPERTIES AND STRUCTURES — $530,000 — 01-3
D. O. Welch, M. Suenaga, C. S. Pande, D. Dew-Hughes

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.

82. PHYSICAL METALLURGY OF METAL HYDRIDE SYSTEMS — $150,000 — 01-3
M. Pick, D. O. Welch, D. Dew-Hughes

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.

83. MATERIALS FOR ELECTROCHEMICAL ENERGY CONVERSION AND STORAGE — $40,000 — 01-3
W. E. O'Grady, S. Srinivasan

The role played by the structure, chemical composition and oxidation states of the surface in electrochemical reactions is being investigated. Surface science techniques including low-energy electron diffraction (LEED), Auger electron spectroscopy (AES) and x-ray photoelectron spectroscopy (XPS) are being combined with electrochemical techniques to study electrocatalysis and other electrochemical reactions on single crystal and alloy surfaces. In combination with these studies experiments are also being carried out on high surface area catalysts in an effort to bridge the gap between studies on well defined single crystal surfaces and those on microcrystal particles.

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

84. RADIATION DAMAGE — $210,000 — 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.

85. EFFECT OF MICROSTRUCTURE AND ENVIRONMENT UPON FRACTURE TOUGHNESS — $180,000 — 01-5
A. Arbel, S. K. Hwang

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

86. NEUTRON SCATTERING - MAGNETIC SYSTEMS — $577,000 — 02-1
S. M. Shapiro, J. D. Axe, C. R. Fincher, Jr., I. U. Heilmann, G. Shirane

Neutron scattering studies of the structure and dynamics of magnetic materials. Spin dynamics of low-dimensional antiferromagnets and amorphous ferromagnets; excitations of itinerant ferromagnets; magnetic ordering in superconductors.

87. NEUTRON SCATTERING - PHASE TRANSITIONS — $625,000 — 02-1
G. Shirane, J. D. Axe, S. K. Satija, S. M. Shapiro, R. Youngblood

Neutron scattering studies of structural phase transitions and their dynamics; low-dimensional charge density waves; phase transitions and dynamics of mercury chain compounds; soft modes in solids.

88. NEUTRON SCATTERING - ELEMENTARY EXCITATIONS IN SOLIDS — $577,000 — 02-1
J. D. Axe, J. Eckert, L. Passell, G. Shirane, W. Thomlinson

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 perovskites.

89. NEUTRON SCATTERING - PARTIALLY ORDERED SYSTEMS — $625,000 — 02-1
L. Passell, J. Eckert, C. F. Majkrzak, S. M. Shapiro, R. Youngblood

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.

BROOKHAVEN NATIONAL LABORATORY
Department of Physics -02-

90. EXPERIMENTAL RESEARCH - SPECTROSCOPY OF SOLIDS — $266,000 — 02-2
B. C. Frazer, Y. Fujii, J. B. Hastings, M. Howells, W. Thomlinson, G. Williams

X-ray and neutron studies of structural, dynamic and electronic properties of solids. Diffuse scattering in ferroelectric phase transitions. 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.

91. EXPERIMENTAL RESEARCH - NATIONAL SYNCHROTRON LIGHT SOURCE, R&D — $916,000 — 02-2
A. van Steenbergen, K. Batchelor, B. C. Frazer, 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)

92. EXPERIMENTAL RESEARCH - PROPERTIES OF REAL SOLIDS — $436,000 — 02-2
A. N. Goland, K. G. Lynn, J. E. Dickman, J. Jean, P. W. Levy, C. L. Snead, Jr. (DEE)

Investigations of perfect and imperfect solids by specialized experimental methods; slow-positron behavior at and near well-characterized metal surfaces, 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, geophysical applications of mineral thermoluminescence; use of EXAFS to study impurities in dilute alloys and valence fluctuations in intermetallics.

93. EXPERIMENTAL RESEARCH - ADVANCED MATERIALS SYNTHESIS AND CHARACTERIZATION — $124,000 — 02-2
A. N. Goland, D. E. Cox, A. Moodenbaugh, J. B. Hastings, B. C. Frazer

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 with emphasis on perovskite structures; application of profile refinement methods to complex oxide structures; structural studies of defects in A-15 superconductors; energy-dispersive x-ray diffractometry, use of EXAFS for defect structure determinations.

94. EXPERIMENTAL RESEARCH - ALTERATION AND ANALYSIS OF SOLIDS BY ION BEAMS — $124,000 — 02-2
A. N. Goland, J. S. Rosner; C. Clayton, H. Herman (SUNY-Stony Brook)

Channeling, Rutherford backscattering, 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, medium-energy proton backscattering, ESCA, and TEM analysis; hydrides, superconductors; surface phenomena and thin films.

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

95. THEORETICAL RESEARCH $547,000 02-3
V. J. Emery, J. Black,
M. Blume, J. Davenport,
G. J. Dienes, G. Reiter,
R. H. Swendsen, R. E. Watson,
G. Wendin

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.

96. PARTICLE-SOLID INTERACTIONS - RADIATION EFFECTS RESEARCH $549,000 02-4
A. N. Goland, P. W. Levy,
K. G. Lynn, K. J. Swyler (DEE),
C. L. Snead, Jr. (DEE),
R. W. Klaffky, Yu. M. Platov (USSR)

Comparison of radiation effects as a function of incident neutron energy spectrum by positron-annihilation lifetime and Doppler-broadening measurements, in situ studies of electron bombardment natural and synthetic NaCl by measurements of optical absorption and radioluminescence; thermoluminescence of gamma-irradiated quartz; dislocation generation in gamma-irradiated crystals; calculation of radiation damage parameters for metals and nonmetals in a deuteron-stripping type intense neutron source.

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

97. ENGINEERING PHYSICS - SUPERCONDUCTIVITY — $446,000 — 02-5
A. Ghosh, Z. Ovadyahu, M. Strongin, H. Wiesmann

Investigations of the density of states, T_c, and transport properties in A-15 superconductors in different states of disorder; tunneling into N-S layers and theory of tunneling into N-S layers; superconductivity in ultra-thin film superconductors and the nature of the superconducting transition in two dimensions.

98. ENGINEERING PHYSICS - SURFACE STUDIES — $188,000 — 02-5
M. El-Batanouny, R. J. Smith, M. Strongin, S. L. Weng

Use of photoemission to determine the properties of hydrogen and other adsorbates on transition metals; studies of different surface overlayers (such as Pd, Ni and Pt) and their effect on hydrogen uptake in niobium and tantalum; studies of overlayer structure and structural transitions in overlayers and how hydrogen uptake in the underlying metal is affected; design and construction of spherical analyzer, beam line, and chamber for photoemission spectroscopy 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

99. 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.

100. WELDING RESEARCH — $200,000 — 01-5
J. F. Key, G. R. Smolik

Heat source/molten pool interaction studies utilizing high-speed cinematography, emission spectroscopy and infrared thermography. Post weld embrittling mechanisms; cracking tendency determinations; age hardenable nickel base alloys; influence of oxygen in the embrittlement process; publication of BES Newsletter; Annual BES Contractors Meeting at INEL.

ILLINOIS, UNIVERSITY OF
Urbana, Illinois 61801

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

101. CHARACTERIZATION OF COMPOUNDS AND ALLOYS — $ 135,000 — 01-1
H. L. Fraser and C. A. Wert

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.

102. THEORY OF POLYMERS — $ 25,000 — 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.

103. DYNAMICAL STRUCTURE OF MATERIALS UNDER EXTREME CONDITIONS OF TEMPERATURE AND PRESSURE — $ 135,000 — 01-1
J. Jonas

Dynamical structure of water and electrolytes at high temperature and pressure. Phase transformation in disordered organic solids; structure-property relationships in polymeric materials. Laser Raman scattering and nuclear magnetic resonance at high temperatures and pressures.

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

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

105. MECHANICAL PROPERTIES OF MATERIALS — $ 50,000 — 01-2
J. Holder

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.

ILLINOIS, UNIVERSITY
Materials Research Laboratory (Continued)

106. RESOURCE COUNCIL ON MATERIALS SCIENCE — $ 50,000 — 01-2
R. J. Maurer

Information and concept resource on current and proposed basic research activities in the area of materials properties and their application to the solution of problems in energy utilization.

107. MECHANISMS OF STRESS-CORROSION CRACKING — $ 60,000 — 01-2
E. N. Pugh

Investigation of intergranular and transgranular crack propagation in engineering materials using fractographic (SEM, TEM) metallographic and acoustic-emission measurements. Role of hydrogen in cracking process.

108. LOCALIZED CORROSION OF PASSIVE METALS — $ 60,000 — 01-3
R. C. Alkire

Corrosion of metals owing to fluid flow. Erosion by particle impaction and cavitation. Transport models of crevice corrosion and differential aeration systems.

109. OXYGEN IN REFRACTORY BCC METALS — $ 40,000 — 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.

110. SOLID DIELECTRICS — $ 70,000 — 01-3
D. A. Payne

Fabrication, characterization and physical property measurements on new and improved piezo, ferro and pyroelectric ceramics for dielectric and energy conversion applications. Microstructure and compensation in diphasic mixtures. Mechanisms of electrode and insulator deterioration under severe electrochemical environments in MHD generation.

111. GRAIN BOUNDARIES IN CERAMICS — $ 10,000 — 01-3
W. T. Petuskey

Segregation and exsolution of impurities and elemental components at grain boundaries during grain growth and phase separation.

ILLINOIS, UNIVERSITY
Materials Research Laboratory (Continued)

112. ELECTRONIC PROPERTIES OF ORGANIC SEMICONDUCTORS — $ 35,000 — 01-3
T. J. Rowland

Electrical, magnetic and magnetic resonance investigation of doped one-dimensional organic semiconductors and hydrogen in BCC metals.

113. SITE LOCATIONS IN CERAMIC MATERIALS — $ 60,000 — 01-3
H. J. Stapleton

Investigations of mobile cation distribution in solid electrolytes and of active sites on rare earth oxide catalysts, using electron-spin resonance and electron-nuclear double resonance methods.

114. PHYSICAL PROPERTIES OF OXIDE CERAMICS — $ 30,000 — 01-3
G. P. Wirtz

Electrical conduction and oxygen mobility in nonstoichiometric oxides for solar energy collection, for oxygen permeable conductors in fuel cells, and for water electrolysis applications. Catalysis by mixed lanthanum-cobalt oxides.

115. LOW TEMPERATURE STUDIES OF DEFECT STRUCTURE IN SOLIDS — $ 110,000 — 02-2
A. C. Anderson

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

116. RESPONSE OF SOLIDS TO ELECTROMAGNETIC RADIATION — $ 60,000 — 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.

117. USE OF VERY HIGH PRESSURES TO INVESTIGATE THE STRUCTURE OF MATTER — $ 145,000 — 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 and effects on luminescence.

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (Continued)

118. EXCITON COLLECTION FROM ANTENNA SYSTEMS INTO ACCESSIBLE TRAPS — $ 30,000 — 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.

119. IMPURITIES IN SUPERCONDUCTORS — $ 50,000 — 02-2
D. M. Ginsberg

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

120. ULTRASONIC INVESTIGATIONS OF THE STRUCTURE OF MATTER — $ 145,000 — 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.

121. PROPERTIES OF CRYSTALLINE CONDENSED GASES — $ 100,000 — 02-2
R. O. Simmons

Phase transitions in solid hydrogen and methane crystals; thermal and isotopic defects in helium crystals; quantum effects in diffusion. Thermodynamics of highly anharmonic insulators from low temperature to melting.

122. DEFECT PROPERTIES OF SOLIDS — $ 90,000 — 02-2
D. Lazarus

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

123. NUCLEAR MAGNETIC RESONANCE IN SOLIDS — $ 155,000 — 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.

ILLINOIS, UNIVERSITY
Materials Research Laboratory (Continued)

124.	PHYSICAL PROPERTIES OF TRANSITION METAL CARBIDES W. S. Williams	$ 75,000	02-2

Investigation of ceramic properties including catalytic behavior of tungsten carbide, effect of order on superconductivity in niobium carbide, hardness microstructure and potential use in photovoltaic conversion of transition metal carbides.

125.	RADIATION DAMAGE IN SOLIDS J. S. Koehler	$ 120,000	02-4

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
D. A. Shirley - Phone: (FTS) 451-5619, or 415/486-5619

126. ATOMIC RESOLUTION MICROSCOPY — $ 48,000 — 01-1
R. Gronsky

Development and use of the most sophisticated electron-optical imaging techniques to photograph atoms in crystalline or amorphous arrangements. Real-space structural analysis. Determination of localized atomic configurations responsible for solid state reactions, bulk as well as surface properties, and materials performance in the new energy technologies.

127. MICROSTRUCTURE, PROPERTIES, ALLOY DESIGN: INORGANIC MATERIALS — $435,000 — 01-1
G. Thomas

Relationships between microstructure and properties; control of properties through characterization and control of structure; application of principles of strengthening and phase transformations to alloy design for mechanical 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.

128. 1.5 MeV ELECTRON MICROSCOPE — $145,000 — 01-1
K. H. Westmacott

Crystal lattice defect-impurity interactions, structural transitions. High voltage electron microscopes equipped with environmental cells are used to conduct dynamic in-situ studies of gas-solid interactions. The object of this research is to understand in detail the changes in microstructure and properties of materials exposed to contamination or hostile environments.

129. THEORETICAL PROBLEMS IN ALLOY DESIGN — $408,000 — 01-2
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 Research Division (Continued)

130. STRUCTURE-PROPERTY RELATIONSHIPS IN SEMICONDUCTOR MATERIALS — $231,000 — 01-2
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. Characterization of spectrally selective electroplated black chrome surface layers.

131. MECHANICAL PROPERTIES OF CERAMICS — $144,000 — 01-2
A. G. Evans

Study of concurrent deformation and fracture processes in ceramic polycrystals at elevated temperatures, to relate these properties to microstructure and local chemistry. Investigation of the microstructural causes of toughening, by correlating crack extension with the effects (transformation, microcracking) that occur within the crack tip process zone. The studies involve modelling, observations of the deformation and fracture sequence, and the characterization of relevant microstructural details at high resolution, using electron microscopy.

132. SUPERCONDUCTIVITY EFFECTS - HIGH FIELD SUPERCONDUCTIVITY — $141,000 — 01-3
J. W. Morris, Jr., and J. L-F. Wang

Application of the principles of materials science to the design of special processing systems that will yield multifilamentary superconducting tape or wire. The filaments are composed of A-15 compounds such as Nb_3Sn, Nb_3Al, $Nb_3(Al,Ge)$ and Nb_3Ge. All of these compounds are extremely brittle and therefore difficult to obtain in the required form of tape or wire. The technical approach emphasized the use of powder metallurgy. Other approaches are used when circumstances favor doing so. Examples are the use of high temperature solid solubilities and preferential precipitation sites such as regions of high strain energy.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

133. INTERFACES AND CERAMIC MICROSTRUCTURES — $225,000 — 01-3
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 constitutents are within the Al_2O_3-SiO_2 system. Thermodynamic considerations of sintering with and without a liquid phase. Relationship to the character (particularly grain boundaries) of ceramic materials to their mechanical behavior at elevated temperatures. Mechanisms of corrosion of ceramic materials. Thermodynamics and kinetics of electrochemical reactions at glass-metal and ceramic-metal interfaces.

134. HIGH TEMPERATURE REACTIONS — $225,000 — 01-3
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 by iron oxides, the catalysis of SO_3 gas decomposition and other reactions by solid surfaces.

135. CHEMICAL PROPERTIES OF CERAMIC ALLOYS AND PROCESSING OF CERAMIC MATERIALS — $100,000 — 01-3
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. Study of the relationship between microstructure, current density, and properties of fast ion conductors. Breakdown is studied by a variety of techniques including various microscopy methods as well as acoustic emission analysis.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

136. STRUCTURE AND ELECTRICAL PROPERTIES OF COMPOSITE MATERIALS — $105,000 — 01-3
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. Mechanism of graphitization and point defect annealing in Glassy Carbon and Pyrolytic Graphite. Composition: aligned two phase microstructures obtained by directional solidification of eutectic alloys. Effect of microstructure on electrical, thermophysical and mechanical properties. Usefulness of rule of mixtures as a predictor.

137. HIGH TEMPERATURE OXIDATION AND CORROSION OF MATERIALS — $295,000 — 01-3
D. P. Whittle

Determination of the effects of metallurgical and environmental variables on the surface degradation of materials in complex gaseous atmospheres and the influence of sulphatic deposits. Mechanisms of degradation, and their relation to diffusional, structural and compositional parameters of the metal oxides, sulfides and carbides involved. Development of resistant materials and coatings; rare earth metal additions to promote improved scale/alloy adherence by modification to the scale/alloy interface; the nature of the alloy/scale interface and optimization of addition elements. Multicomponent diffusion studies in coating/alloy substrate systems and quantitative relationship to the fundamental thermodynamic and transport properties involved.

138. EROSION-CORROSION WEAR PROGRAM — $400,000 — 01-5
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 particle trajectories and erosion mechanisms over a wide range of operating conditions. Establishment of material design criteria for erosion-corrosion resistant materials.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

139. IN-SITU INVESTIGATIONS OF GAS-SOLID REACTIONS BY ELECTRON MICROSCOPY — $ 48,000 — 01-5
J. W. Evans

Use of environmental cells in the existing 650 kV electron microscope and the new 1.5 MeV electron microscope for an investigation of the effect of microstructure on reactions between gases and solids. Nickel oxide reduction by hydrogen, which shows evidence of being strongly influenced by microstructure will be studied first; subsequently, oxidation, sulfidation and other reactions of significance to materials performance in energy conversion systems will be investigated.

140. FAR INFRARED SPECTROSCOPY — $188,000 — 02-2
P. L. Richards

Development of improved types of far infrared detectors, mixers, and spectrometers. Use of advanced infrared techniques for the measurement of: the vibrational frequencies of molecules chemically adsorbed on metal surfaces, 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.

141. EXPERIMENTAL SOLID STATE PHYSICS AND QUANTUM ELECTRONICS — $222,000 — 02-2
Y. R. Shen

Modern optical techniques are used to study linear and nonlinear optical properties of materials. The materials under investigation include gases, liquids, liquid crystals, metals, semiconductors, and magnetic crystals. Newly-developed optical techniques are applied to current problems of interest, such as laser isotope separation, photochemistry, and surface phenomena.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

142. EXCITED QUANTUM FLUIDS IN SOLIDS $143,000 02-2
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 system, and the possible transient existence of biexcitons and higher excitonic molecules during the nucleation of the liquid.

143. SUPERCONDUCTIVITY, SUPERCONDUCTING DEVICES, AND 1/f NOISE $218,000 02-2
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; enhancement of the energy gap by tunnel injection; response of superconducting films to pulsed perturbations; measurement of the electron-phonon relaxation times in aluminum, tin, and lead.

144. TIME-RESOLVED SPECTROSCOPIES IN SOLIDS $ 0 02-2
P. Y. Yu

The purpose of this program is to develop an optical system capable of measuring the absorptivity, reflectivity, photoluminescence, Raman and Brillouin spectra of a sample as a function of time with the precision of a few picoseconds. This system will be utilized to study the following problems: Relaxation of hot carriers in semiconductors via carrier-carrier interaction and carrier-photon interaction; the temporal behavior of Raman and Brillouin scattering in solids as the excitation frequency is varied from the non-resonant regime to the resonant regime; transient optical response in solids exhibiting spatial dispersion effects (such as in the vicinity of an exciton-polariton in semiconductors); transient photoconductivity in semiconductors with deep traps, and picosecond nonlinear spectroscopies in solids.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

145. THEORETICAL SOLID STATE PHYSICS $ 59,000 02-3
M. L. Cohen

A variety of theoretical approaches aided by computer calculations are used to explain measured properties and to predict new properties of solids: surface energy states on clean semiconductors and transition metals; adsorbates on solids; electrons at interfaces (Schottky barriers and heterojunctions); bulk electronic properties of semiconductors and transition metals; phonon and nonphonon mechanisms for superconductivity and properties of high transition temperature A15 superconductors; development of pseudopotential theory.

146. THEORETICAL STUDIES OF THE ELECTRONIC PROPERTIES OF SOLID SURFACES $ 0 02-3
L. M. Falicov

Theoretical studies of: (A) The structural properties of surfaces, namely the organization and arrangement of atomic constituents at equilibrium; (B) The constitutional properties of the surface, in particular the segregation properties of alloys at the surface as a function of crystal structure, surface orientation, nominal chemical composition and temperature; (C) The electronic structure of surfaces, in particular electron states and electron densities in the neighborhood of the surface; (D) The vibronic properties of surfaces; (E) The magnetic properties of surfaces, both in magnetic solids (ferromagnetic and antiferromagnetic) or in nonmagnetic solids which may develop a magnetic surface layer; (F) The chemical--in particular the catalytic--properties of solids as they are related to the basic physical properties (A)-(E).

147. HIGH PRESSURE CHEMISTRY $ 19,000 03-1
G. Jura

Objectives: Determination of the heat capacities of metals and alloys as a function of temperature and pressure; determination of heat conductivities of nonmetals as a function of temperature and pressure; heats of polymorphic transitions. Use of the heat capacities as a means of deducing the equation of state-of-the metal or alloy under consideration, and for the characterization of the thermodynamic properties. Development of pulse methods on the microsecond scale.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

148. LOW TEMPERATURE PROPERTIES OF MATERIALS — $123,000 — 03-1
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 susceptibitlity 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.

149. ELECTROCHEMICAL PROCESSES — $123,000 — 03-1
C. W. Tobias

This program is designed to advance the scientific foundations of electrochemical engineering, and to widen the range of useful applications of electrochemical transformations. Mass and charge transport in cell processes: combined influences of electrode geometry, surface potential, and ionic transport on the distribution of current on electrode 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.

150. SYNTHESIS, MORPHOLOGY AND PROPERTIES OF HIGH PERFORMANCE POLYMERIC MATERIALS — $ 0 — 03-2
M. M-C. Shen (deceased)

The purpose of this project is to carry out the synthesis of new polymeric materials by the technique of plasma initiation. These new materials will be characterized by a variety of methods, such as electron microscopy; electron, infrared, nmr and ultraviolet spectroscopies; gel permeation chromatography, and electron and neutron scattering. The polymers will be studied to identify their molecular and supramolecular structures, their mechanical, thermal and viscoelastic properties, their Grüneisen functions, and significant correlations. Emphasis will be placed on such polymers as ultrahigh molecular weight organic, organometallic, inorganic and "polymeric alloys". These combinations of polymers will utilize the techniques of block and graft copolymer synthesis.

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

151. HIGH TEMPERATURE THERMODYNAMICS — $103,000 — 03-3
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 characterization of phase boundaries. The data are being used to test and improve chemical models capable of predicting the thermodynamic properties of high-temperature materials.

152. CHEMISTRY AND MATERIALS PROBLEMS IN ENERGY PRODUCTION TECHNOLOGIES — $177,000 — 03-3
D. R. Olander

Chemical and physical behavior of materials in environments characteristic of energy production devices, with major emphasis on fission and fusion reactors. Experiments are designed to develop insight into the mechanisms of the phenomena involved: the high temperature behavior of uranium dioxide, including transient vaporization, oxygen self-diffusion, thermal gradient migration of 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.

153. PLASMA-ENHANCED DEPOSITION OF THIN FILMS — $ 44,000 — 03-3
D. W. Hess

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

154. ELECTROCHEMICAL PHASE BOUNDARIES — $138,000 — 03-3
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.

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

155. SOLID STATE AND SURFACE REACTIONS — $280,000 — 03-3
G. A. Somorjai

Studies of the structure, chemical composition and oxidation state of surfaces and of adsorbed gases using low-energy electron diffraction and various techniques of electron spectroscopy. Investigations of chemical surface reactions and catalysis on crystal surfaces at low and at high pressures by jointly using several techniques: molecular beam scattering, gas chromatography and mass spectrometry.

156. NUCLEAR MAGNETIC RESONANCE — $123,000 — 03-3
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 LABORATORIES
P. O. Box 808
Livermore, California 94550

G. Dorough - Phone: (FTS) 532-4892 or 415-422-4892
L. Roberts - Phone: (FTS) 532-6340 or 415-422-6340

157. HOT CORROSION STUDIES RELATED TO FOSSIL FUELS — $170,000 — 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; effects of oxide additions to a given salt. Potentiostatic and potentiokinetic polarization of nickel and its alloys in molten sodium sulfate.

158. RAPIDLY QUENCHED AMORPHOUS MATERIALS RESEARCH — $ 90,000 — 01-3
B. Holt, C. Cline

Selection, preparation and preliminary screening of beryllium base glassy metal alloys via melt spinning technique. Characterization by scanning calorimetry, and hardness measurements.

159. LOW INDEX OPTICAL MATERIALS RESEARCH — $221,000 — 02-2
M. J. Weber, C. Cline,
W. L. Smith

Nonlinear optical properties of materials subjected to intense light beams; intensity-dependent refractive index change and multiphoton absorption; optical materials studies include: glasses (fluorides, oxides), crystals (alkali halides, oxides), and polymers; time-resolved interferometry used to measure nonlinear refractive index.

160. OPTICALLY-INDUCED DAMAGE IN TRANSPARENT DIELECTRIC MATERIALS — $ 98,000 — 02-2
D. Milam, W. H. Lowdermilk,
A. Rosencwaig

Laser damage in transparent dielectric materials as a function of pulse duration (100 ps - 30 ns) and wavelength at (1064 nm, 532 nm, 355 nm, and 266 nm); materials include optical glasses, alkali halide and oxide crystals; and thin film; studies of electron avalanche, multiphoton absorption, bulk absorption, surface properties, and nonlinear absorption.

LAWRENCE LIVERMORE LABORATORY (continued)

161. LASER-EXCITED FLUORESCENCE IN AMORPHOUS SOLIDS — $ 98,000 — 02-2
M. J. Weber, S. Brawer

Laser-induced fluorescence line narrowing to probe variations in local fields and ion-phonon interactions of paramagnetic ions in disordered solids. Simple and multicomponent oxide and fluoride glasses. Computer simulations of glass configurations using Monte Carlo methods. Modeling of local ion coordination and structure.

162. THIN FILM MATERIALS STUDIES FOR LASER OPTICAL COATINGS — $113,000 — 02-2
J. Khan

To develop a quantitative understanding of the factors that influence the properties of thin film; clarification of the relationship between deposition process variables and atomic scale structure employing scanning high energy electron diffraction; effects of stress, diffusion, annealing and recrystallization; TiO_x.

163. CRYOGENIC D-T PROPERTIES (Formerly D_2-DT-T_2 Phase Diagram) — $160,000 — 03-2
P. C. Souers

This program is currently concentrating on chemical and ortho-para rates of D_2, DT, and T_2, as measured by infrared and nuclear magnetic resonance spectroscopy. New, radiation-induced infrared lines are also being studied. A sizeable experiment on the electrical properties of D-T gas has been completed. Upcoming work includes the gas-phase reaction rates and the solid thermal conductivity.

164. SURFACE PHYSICS AND CHEMISTRY OF LASER INDUCED DAMAGE — $110,000 — 02-2
W. H. Lowdermilk, W. J. 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.

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

Chemistry - Materials Science Division
W. J. Maraman - Phone: (FTS) 843-4563 or 505-667-4563
M. G. Bowman - Phone: (FTS) 843-6014 or 505-667-6014

165. HIGH TEMPERATURE MATERIALS FOR ENERGY APPLICATIONS — $190,000 — 01-3
E. K. Storms, B. A. Mueller

Knudsen and Langmuir vaporization of various rare earth borides; boron and metal activities determined by high temperature mass spectrometry; data used to obtain vapor composition, surface composition, mass loss rate, phase relationship, thermodynamic properties and a general model of vaporization for similar materials; data is being applied to give a proper interpretation to the electron emission behavior when the hexaborides are used as electrodes in thermionic diodes; a search is being made to find ternary boride emitters which are better than LaB_6.

166. RADIATION EFFECTS STUDIES FOR ADVANCED ENERGY TECHNOLOGIES — $300,000 — 01-4
J. R. Cost, W. V. Green
D. M. Parkin, W. F. Sommer

800 MeV proton (LAMPF) irradiation of Aℓ under cyclic stressing; interaction of radiation damage and mechanical damage; analysis of radiation damage under pulsed irradiation; damage analysis in polyatomic materials; radiation effects in amorphous metals; differential cross section measurements of radiation damage in Cu and Pt by dislocation damping.

167. MATERIAL DEFORMATION UNDER MULTIAXIAL LOADING — $130,000 — 01-5
S. S. Hecker, J. J. Petrovic
M. Stout, K. Staudhammer
D. L. Rohr

Multiaxial deformation of aluminum, copper and stainless steel; small deformations by biaxial sheet stretching; study of the evolution of microstructure with plastic deformation

LOS ALAMOS SCIENTIFIC LABORATORY
Chemistry - Materials Science Division

168. CTR RELATED CHEMICAL RESEARCH TRITIUM CHEMISTRY ASSOCIATED WITH THE LITHIUM BLANKET AND CONTAINER MATERIALS — $150,000 — 03-2
D. H. W. Carstens, J. L. Anderson

Solubility measurements of container materials (e.g. Ta, Mo and W) in both La_5Nu and Li over the temperature range 700 to 1100 K; studies of the removal of tritium by La_5Ni from helium streams as a function of flow rate and temperature in the PPM range of tritium.

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

169. MATERIALS RESEARCH ON THE LOS ALAMOS SPALLATION NEUTRON SOURCE — $350,000 — 02-1
T. A. Kitchens, R. Fluharty, P. Seeger, J. Yarnell, J. Eckert P. Vergamini, R. Silver

Development of instrumentation to utilize the special characteristics of the new pulsed spallation neutron source at Los Alamos for materials research; the initiation of an inelastic scattering spectroscopy of adsorbed molecules and hydrogen contained in materials; spectrometer design and construction of a small angle neutron scattering spectrometer for non-destructive evaluation of polymers, irradiated materials, and biomaterials; elastic scattering spectrometer development and utilization on amorphous and powdered crystalline specimens; and assessment of spectrometer characteristics for single crystal investigations.

170. ULTRAHIGH PRESSURE STUDIES OF HYDROGEN — $130,000 — 02-2
R. L. Mills, D. H. Liebenberg

Measure simultaneously pressure, volume, temperature, and ultrasonic velocity in pure cryogenic gases and their mixtures using a piston-cylinder apparatus to 40 kbar; carry out spectral and scattering studies on gases to 500 kbar in diamond-anvil cells; devise techniques for loading diamond cells with high-density helium as a pressure transmitting medium to hundreds of kilobars; develop multistage systems that combine diamond cells with other pressure devices to reach 1 Mbar in the hydrogen isotopes.

LOS ALAMOS SCIENTIFIC LABORATORY
Theoretical Division
P. Carruthers - Phone: (FTS) 843-4401 or 505-667-4401

171. ELASTIC WAVE SCATTERING AND QUANTITATIVE FLAW IDENTIFICATION — $130,000 — 01-5
J. E. Gubernatis, W. M. Visscher
G. A. Baker, Jr.

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.

172. LOS ALAMOS EQUATION OF STATE LIBRARY — $220,000 — 02-3
G. I. Kerley, B. I. Bennett,
J. D. Johnson, R. C. Albers,
S. P. Lyon

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 caluclations and other applications. Distribute data to users on magnetic tape in a universal computer format. Apply theories of solids, liquids, gases, plasmas, and mistures to generation of EOS data. Develop new theoretical methods when existing theories and experiments are insufficient to satisfy user requirements.

Accelerator Technology Division
E. Knapp - Phone: (FTS) 843-2060 or 505-667-2060

173. PROTON STORAGE RING R&D PROGRAM — $200,000 — 02-1
G. P. Lawrence, G. Spalek,
R. Higgins, M. Barbier,
A. Jason, R. Cooper

Shielding calculations to determine adequate protection from high energy neutrons produced by various modes and amounts of proton beam loss at high current operation; design study of large aperture storage ring magnet prototypes, both dipole and quadrupole; design and development of reusable, remote-handling-compatible, high vacuum couplings; measurements to estimate effects of beam induced electron multipactoring at high currents; bunched beam calculations at high space charge levels.

MOUND LABORATORY
P. O. Box 32
Miamisburg, Ohio 45342
W. H. Smith - Phone: (FTS) 774-7296 or 513-866-7296

174. SOLAR ENERGY FLUIDS $240,000 01-3
L. J. Wittenberg

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; thermal storage materials for use above 200°C based upon complex fused salts and liquid metal alloys; selected thin film studies.

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
J. O. Stiegler-Section Head - Phone: (FTS) 624-5052 or 615-574-5052

175. THEORETICAL STUDIES OF METALS AND ALLOYS $350,000 01-1
J. S. Faulkner, W. H. Butler, J. F. Harris,
G. S. Painter, G. M. Stocks

Local density formalism (LDF) combined with cluster program and layer KKR program to study electronic states of surfaces and energetics such as binding energy of adsorbates, surface molecular dissociation, and chemical properties of reaction intermediates; 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.

176. X-RAY SCATTERING RESEARCH $240,000 01-1
H. L. Yakel, B. S. Borie,
R. W. Hendricks, C. J. Sparks

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

177. PREPARATION AND SYNTHESIS OF HIGH TEMPERATURE MATERIALS $360,000 01-1
G. W. Clark, C. B. Finch,
J. D. Holder, C. F. Yen

Directionally solidification of binary and ternary non-metal matrices-systems (oxides, carbides, borides) which contain a metal(s); preparation and evaluation of directionally solidified WC-Co, TiB_2-TiC, ZrO_2 (Y_2O_3)-Al_2O_3(Cr_2O_3)-Mo, and liquid phase sintered TiB_2-Fe(Ni) and $(Ti,X)B_2$-Fe(Ni) for tool and wear applications; theoretical treatment of coupled transport phenomena in crystal growth; actinide-doped crystals; quartz; growth of single crystals of carbides and nitrides.

178. STRUCTURE OF COAL $ 90,000 01-1
L. A. Harris, C. S. Yust

TEM, SEM, microprobe, optical and infrared petrography of microporosity and microminerology of coal macerals; correlation of coal rank with microstructure; characterization of secondary minerals in microfractures; anthracite, bituminous, sub-bituminous, and channel coals.

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

179. SHAPE MEMORY EFFECT IN URANIUM ALLOYS — $240,000 — 01-1
R. A. Vandermeer, J. C. Ogle

Pseudoelasticity and shape memory effects in U-Nb-Zr, U-Nb, and U-Ti alloys; relation between thermoelastic martensite and deformation; interaction of impurities with thermoelastic martensite phase boundaries; strain recovery kinetics.

180. X-RAY RESEARCH USING SYNCHROTRON SOURCES — $ 90,000 — 01-1
C. J. Sparks, H. L. Yakel

Development and use of fluorescence, anomalous dispersion, and scattering techniques for x-rays at the Stanford Synchrotron Radiation Laboratory; design and construction of beam line for installation at the National Synchrotron Light Source, Brookhaven National Laboratory; long- and/or short-range order in Fe-Ni-Cr alloys; atom positions in sigma phase and Fe-Co spinels.

181. HIGH VOLTAGE AND ANALYTICAL ELECTRON MICROSCOPY — $250,000 — 01-1
R. W. Carpenter, J. Bentley, E. A. Kenik, N. Zaluzec

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.

182. DEFORMATION AND MECHANICAL BEHAVIOR OF STRUCTURAL MATERIALS — $470,000 — 01-2
M. H. Yoo, K. Farrell, T. C. Reiley, R. A. Vandermeer, C. L. White

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.

183. KINETICS AND MECHANISMS OF SURFACE AND SOLID STATE REACTIONS — $500,000 — 01-3
J. V. Cathcart, P. T. Carlson, 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; theoretical and experimental studies of high temperature oxidation of Zr and its alloys; diffusion mechanisms and solute-lattice interactions for interstitials in oxides (T in TiO_2, Al_2O_3, Cr_2O_3); diffusion in sulfur-doped oxides; mechanisms of fast diffusion in lead alloys.

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

184. PHYSICAL PROPERTIES RESEARCH — $325,000 — 01-3
D. L. McElroy, R.O.A. Hall, 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) and transition metals (Fe, Cr); phonon-phonon scattering in insulating solids having NaCl, CaF_2 and CsCl structures, effect of cation-anion mass ratio, grain boundaries and crystal structure; properties of LRO alloys; low temperature properties of polymers used in superconducting magnets.

185. SUPERCONDUCTING AND AMORPHOUS/METASTABLE MATERIALS — $405,000 — 01-3
C. C. Koch, A. DasGupta, D. S. Easton, D. M. Kroeger, W. Specking

Flux pinning in Nb-Hf, Nb_3Sn and bicrystals of V_3Si; stress/strain effects on superconducting parameters of Nb_3Sn and V_3Ga; amorphous superconductors based on Mo, La, Re, and Nb with other transition metals and/or metalloids, influence of magnetic impurities on paramagnetic limit of H_{C2}; arc-hammer, electron-beam vapor deposition, and ion-implantation techniques.

186. RADIATION EFFECTS — $1,200,000 — 01-4
L. K. Mansur, W. A. Coghlan, K. Farrell, G. R. Gessel, E. A. Kenik, M. B. Lewis, N. H. Packan, T. C. Reiley, M. R. Hayns, J. E. Harris, W. Kesternich

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, Mg and alloys, stainless steels, LRO alloys.

187. EROSION AND WEAR OF CERAMICS — $ 90,000 — 01-5
C. S. Yust, C. F. Yen

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.

OAK RIDGE NATIONAL LABORATORY
Metals and Ceramics Division -01- (Continued)
J. Slaughter - Section Head - Phone: (FTS) 624-3983

188. FUNDAMENTAL STUDIES IN WELDING $370,000 01-5
G. M. Goodwin, S. David,
J. M. Leitnaker

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

189. 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

190. ELEMENTARY EXCITATIONS IN CONDENSED MATTER — $665,000 — 02-1
R. M. Nicklow, J. W. Cable, W. C. Koehler, R. D. Lowde, H. A. Mook, Y. Noda, C. Perry, H. G. Smith, Y. Yamada, N. Wakabayashi

Inelastic neutron scattering studies of phonons, magnons, and single particle excitations in solids and liquids; lattice dynamics and magnetic excitations in $CeSn_3$, γ-Ce, SmS, and $Sm_xY_{1-x}S$; spin wave spectra in Fe-V and Pd-Fe alloys; spin waves at high energies in Ni; spin waves at high temperatures in Ni; excitations in Gd above the Curie point; phonon measurements and phase transitions in $MEM(TCNQ)_2$, $TiSe_2$, and $Pd_{1-x}Ge_xTc$.

191. MAGNETIC PROPERTIES OF SOLIDS — $475,000 — 02-1
R. M. Moon, J. W. Cable, H. R. Child, W. C. Koehler, H. A. Mook, R. M. Nicklow, R. Parra, N. Wakabayashi

Elastic and inelastic scattering of polarized and unpolarized neutrons by magnetic systems; magnetic moment distributions in the alloy systems Ni-Pt and Pt-Gd; magnetic structure of TmS; magnetic structures of Nd; magnetic moment density in valence fluctuation systems SmS, $Sm_{0.76}Y_{0.24}S$, SmB_6, and $Ce_{0.74}Th_{0.26}$; induced moment form factor and moment density of Zr, Bi, Fe-Cu alloys, $CeSn_3$ and SmN; magnon spectra and lifetimes in rare earth metals and alloys and Laves phase intermetallic compounds.

192. PROPERTIES OF DEFECTS, SUPERCONDUCTORS, AND HYDRIDES — $655,000 — 02-1
W. C. Koehler, H. R. Child, D. K. Christen, H. A. Mook, R. M. Moon, R. M. Nicklow, H. G. Smith, S. Spooner, N. Wakabayashi, G. D. Wignall

Elastic, inelastic and small-angle scattering of neutrons by superconductors, superionic conductors, metal hydrides, thin films, and by elements and compounds containing defects; high resolution neutron spectrometry of KCl(CN); phonon spectra of superconductors, α-U, Mo-Re, A15 type compounds; dynamic properties of tritium in metallic systems; electron-phonon interactions in Nb and Mo; phase transitions in α-U; phonon densities of states, magnetic structures, and magnetic excitations in re-entrant superconductors; localized modes in Th(.06C); diffusion of D in Th and Th(.06C); lattice dynamics and diffusive modes in silver halides; small-angle scattering studies of voids in irradiated metals and irradiated stainless steel; swelling in coals; polymer blends; high resolution small-angle diffraction studies of fluxoid lattice anisotropy in high T_c superconductors.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

193. PHYSICAL PROPERTIES OF SUPERCONDUCTORS $365,000 02-2
S. T. Sekula, B. R. Appleton,
D. K. Christen, H. R. Kerchner,
M. D. Sherrill, J. R. Thompson,
H. W. Weber, 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 in superconductors.

194. PHYSICAL PROPERTIES OF CERAMICS $590,000 02-2
J. B. Bates, E. Sonder,
M. M. Abraham, Y. Chen,
H. L. Engstrom, T. Kaneda,
F. A. Modine, J. C. Wang,
R. A. Weeks

Solid state reactions at high temperatures involving charge and mass transport and valence changes of defects and impurities in materials such as MgO, Al_2O_3, TiO_2, and $MgAl_2O_3$; determination of the mechanisms involved in electric breakdown at high temperatures; mechanisms of hydrogen diffusion; techniques include measurements of electrical conductivity, thermoelectric power, and diffusivities, Raman scattering, polarization modulation and Fourier transform infrared spectroscopy, optical absorption and emission, electron paramagnetic resonance, and electron-nuclear double resonance.

195. RESEARCH AND DEVELOPMENT ON PURE MATERIALS $635,000 02-2
L. A. Boatner, M. M. Abraham,
G. C. Battle, W. E. Brundage,
Y. K. Chang, T. F. Connolly,
M. L. Linvill, M. Rappaz

Growth and characterization of high-quality single crystals of research materials; compilation and dissemination of information regarding the physical properties and worldwide availability of single crystals and research materials by the Research Materials Information Center; growth of single crystals of synthetic minerals ($CePO_4$, $LaPO_4$, YPO_4) for the primary containment of high-level radioactive wastes; growth of single crystals of perovskite-structure oxides ($KTaO_3$, $KTa_{1-x}Nb_xO_3$) and semiconducting oxides for photoelectrochemical cell electrode investigations; float-zone and tri-arc growth of A15 compounds (V_3Si, Ti_3Au, Ti_3Pt), arc-fusion and flux growth of high-temperature materials (WC, Y_2O_3, MgO, CaO, SrO); flux growth of single crystals of fast-ion conductors (β"-alumina), Czochralski and float-zone growth of single crystals of Fe-Cr-Ni alloys (i.e., stainless steels); electron-beam float-zone growth of refractory metals (Ti, V, Zr, Nb, Ta, W, Ir, Re); preparation of high-purity metals and alloys in rod and foil form; growth of CdSe single crystals.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

196. PHOTOPHYSICAL PROCESSES OF SOLAR ENERGY CONVERSION — $485,000 — 02-2
R. F. Wood, B. R. Appleton, J. W. Cleland, H. L. Engstrom, G. E. Jellison, B. C. Larson, J. Narayan, J. C. Wang, 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.

197. FUNDAMENTAL ASPECTS OF METAL FRACTURE — $240,000 — 02-2
S. M. Ohr, S. J. Chang, 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 stainless steel, molybdenum and magnesium oxide; distribution of dislocations in the plastic zone ahead of the crack tip in metals and ceramics; high resolution electron microscope studies of crack nucleation.

198. SOLID ELECTROLYTES AND SUPERIONIC CONDUCTIVITY — $180,000 — 02-2
J. B. Bates, M. M. Abraham, G. M. Brown, W. E. Brundage, H. L. Engstrom, T. Kaneda, B. C. Larson, J. C. Wang

Mechanisms of high ionic conductivity in solid electrolytes such as the beta- and beta"-aluminas; preparation and characterization of new materials based on modification of the beta-alumina structure; proton conduction in beta- and beta"-aluminas; techniques include measurements of electrical conductivity and dielectric constant, Raman scattering, infrared absorption, reflection and emission spectroscopy, x-ray scattering, x-ray diffraction, neutron diffraction, and electron paramagnetic resonance spectroscopy; experimental results interpreted and correlated by means of model calculations.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

199. THEORY OF CONDENSED MATTER $820,000 02-3
R. F. Wood, J. H. Barrett,
J. F. Cooke, H. L. Davis,
L. J. Gray, T. Kaplan,
M. E. Mostoller, O. S. Oen,
M. Rasolt, M. T. Robinson,
M.V.K. Ülehla

Theory of laser annealing and laser-induced diffusion 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 back-scattered ions; interpretation of LEED data; 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; latttice 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.

200. LOW TEMPERATURE RADIATION EFFECTS $465,000 02-4
R. R. Coltman, Jr., C. E. Klabunde,
J. M. Williams, D. B. Poker,
J. K. Redman

Fission-neutron damage rates in metals and alloys at 4.7 K for damage efficiency determinations; magnetoresistance of irradiated Cu and Al for composite superconductors; defect-production studies in alloys and pure and doped metals fast-neutron irradiated near room temperature; normalization of ion and fission-neutron damage in Ni irradiated near 4 K; correlated studies of resistivity and density changes in Cu fast-neutron irradiated near room temperature; effects on insulators for superconducting magnets irradiated at 4.7 K; thermal-neutron production and diffusion of He in Ni; fast-neutron irradiation of Sn-SnO-Sn Josephson junctions at 4.7 K; effect of thermal-neutron irradiation at 4.7 K on the transition temperature of Nb_3Au.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

201. X-RAY DIFFRACTION AND ELECTRON MICROSCOPY — $350,000 — 02-4
T. S. Noggle, J. F. Barhorst, B. C. Larson, J. Narayan, S. M. Ohr

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; laser annealing; 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.

202. ION BOMBARDMENT — $280,000 — 02-4
B. R. Appleton, J. H. Barrett, O. W. Holland, O. E. Schow III, C. W. White, S. R. Wilson, S. P. Withrow, D. M. Zehner, R. A. Zuhr

Development of Positive Ion Crystallography of Surfaces (PICS) technique for surface studies; application of PICS to studies of reordered, relaxed and oxygen covered single crystal surfaces; exploitation of the channeling effect in the narrow and wide (111) planar subchannels in Si to study impact parameter dependent stopping powers of He, C, and B ions; investigations of uni- and bi-directional double alignment channeling for defect studies; 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 and Pt and Pd in Ti and Mo single crystals; measurements of one-dimensional lattice contraction by ion channeling and x-ray scattering; development of nuclear resonance techniques for detecting Al, H_2, and D_2 in solids; investigations of laser annealing mechanisms of defects in Si, Nb, and Al by ion scattering-channeling techniques.

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

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

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

204. SURFACE STUDIES AND CATALYSIS — $565,000 — 02-5
L. H. Jenkins, B. R. Appleton,
J. H. Barrett, H. L. Davis,
M. E. Mostoller, J. R. Noonan,
M. Rasolt, M.V.K. Ulehla,
J. F. Wendelken, D. M. Zehner

Studies of the crystallographic and electronic structure of clean and adsorbate-covered metal 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), and computer simulations for surface crystallography studies; LEED and Auger electron spectroscopy (AES) from "d" and "f" electron band solids; AES of quasi-atomic nature, angular emission dependence and line shape analysis of Auger spectra; vibronic structure of adsorbates examined by high resolution electron energy loss spectroscopy; examination of surface electronic and geometric structures with respect to solid state aspects of heterogeneous catalysis.

205. ION IMPLANTATION — $230,000 — 02-5
B. R. Appleton, E. J. Kelly,
O. E. Schow III, S. T. Sekula,
N. G. Thompson, C. W. White,
S. R. Wilson

Capability for in situ ultra high vacuum ion implantation, ion scattering-channeling and surface analyses, and laser annealing; investigations of laser annealing mechanisms and implanted impurity mobility in ion-implanted silicon; characterization of ion-implanted, laser-annealed silicon for improved efficiency solar cells; 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 of superconducting materials and laser processing; investigations of metastable materials prepared by ion implantation doping and laser processing; studies of metastable alloys and amorphous transitions in ion-implanted, laser-annealed metals; rapid heating and cooling studies; crystal regrowth and solidification phenomena.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

206. RESEARCH AND DEVELOPMENT - ISOTOPE RESEARCH MATERIALS PREPARATION — $280,000 — 02-5
E. H. Kobisk, W. S. Aaron, H. L. Adair, K. Nacke

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 developmental 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

207. CHEMICAL STRUCTURE OF ENERGY RELATED MATERIALS — $780,000 — 03-1
W. R. Busing, G. M. Brown, C. K. Johnson, E. Johnson, A. H. Narten, W. E. Thiessen

Atomic and molecular arrangements in crystals and in liquids determined by neutron and x-ray diffraction studies; precise location of light atoms, especially hydrogen, in crystals; separation of atom-atom pair correlation functions for liquids; development of synchrotron radiation facilities. Advancement of computational methods for solving and refining crystal structures; 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, catalysts for the photochemical production of hydrogen, hydrocarbon liquids and liquid mixtures related to petroleum production, sterically hindered hydrocarbons, and superionic and organic electrical conductors.

208. HIGH TEMPERATURE CHEMISTRY AND THERMODYNAMICS OF STRUCTURAL MATERIALS — $520,000 — 03-2
J. T. Bell, H. F. Bittner, J. Brynestad, J. D. Redman, G. M. Begun

The chemistry and thermodynamics of structural materials at temperatures in the 400 to 1000°C range are investigated; reactions, kinetics and thermodynamics that describe sorption, corrosion and microphase formation are the primary objectives. Sorption studies include hydrogen isotope sorption by both pure metals and alloys. Measurements of tritium permeation rates through strucutral alloys into steam atmospheres are a major effort where the inherent permeabilities of materials, the effects of surface oxidation on the overall permeation process, and the chemical and physical characterization of the oxides are particular interests. These studies already have shown that the amounts and the compositions of the oxides formed by steam oxidation of a given alloy will 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. The formation of microphases also affects the corrosion properties, and this new correlation is also investigated.

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

209. PHYSICAL CHEMISTRY OF MOLTEN SALTS IN ENERGY UTILIZATION — $230,000 — 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; modelling and measurement of polarization and mass transport in electrolytes and electrodes relevant to high temperature battery and fuel cell applications.

210. LOCALIZED CORROSION AND STRESS CRACKING PHENOMENA RELATED TO ENERGY TECHNOLOGIES — $350,000 — 03-3
F. A. Posey, A. L. Bacarella, E. J. Kelley, 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; kinetics of corrosion reactions in concentrated aqueous electrolytes; effect of strain on dissolution kinetics; development of rapid electrochemical methods for testing susceptibility to localized attack.

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

211. THERMODYNAMICS OF ENERGY RELATED SYSTEMS — $205,000 — 03-2
T. B. Lindemer, E. C. Beahm, T. M. Besmann

Fundamental 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); $PuO_{1.5}$-$PuC_{1.5}$-C; $PuO_{1.5}$-$PuC_{1.5}$-Pu(C,O); ThO_2-ThC_2-C; 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.

212. CHEMICAL ENGINEERING RESEARCH — $205,000 — 03-2
J. S. Watson, S. D. Clinton, R. E. Barker

The measurement and evaluation of materials properties important to chemical processes; the development and evaluation of techniques for physical removal of solid particles from viscous fluids (e.g., coal-derived liquids). Present efforts focus on deep-bed filters for removing very small (submicron) particles from organic and aqueous streams.

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

T. D. Chikalla - Phone (FTS) 444-7511 ext. 2576 or 509-946-2576

213. METAL-INSULATOR-SEMICONDUCTOR PHOTOVOLTAICS — $95,000 — 01-1
J. E. Garnier, R. P. Turcotte, L. C. Olsen

Photoelectric and physical/chemical structure evaluation of MIS photovoltaic cells. Correlation of performance to thin film structure/fabrication parameters to improve understanding of basic parameters which control the photovoltaic processes in such cells. Thin film properties--optical transmission, ellipsometry, Auger profile analyses, electron microscopy. Systems of major interest based on single crystal silicon--Au/SiO_x/n-Si and Al/SiO_x/p-Si.

214. SPUTTER-DEPOSITED AMORPHOUS SILICON FOR SOLAR APPLICATION — $60,000 — 01-1
W. T. Pawlewicz, P. M. Martin

Investigate property/composition relationships in sputter-deposited hydrogenated a-Si. Determine optical and electrical properties as a function of H incorporated into the a-Si film as well as the local environment at the H atom in the Si lattice. Investigate the effects of sputtering conditions on film properties and Si-H bonding; optical and IR spectroscopic technique; electrical transport measurements; SIMS, Auger and gas evolution analysis.

215. PHOTOELECTROCHEMICAL PROPERTIES OF SOLAR MATERIALS — $65,000 — 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 metal oxides and semiconductors; effects of natural impurity in plasma-sprayed TiO_2 for photoelectrolysis of water; crystalline and amorphous $SrTiO_3$ and Fe_2O_3-TiO_2 compounds; degradation and corrosion of semiconductor electrodes; and surface modification for enhanced stability.

PACIFIC NORTHWEST LABORATORY (continued)

216. FUNDAMENTAL STUDIES OF STRESS CORROSION AND CORROSION FATIGUE MECHANISMS — $160,000 — 01-2
R. H. Jones, M. T. Thomas, S. M. Bruemmer

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 and experimental measurement of surface and grain boundary segregation of S, P, Sb, C and O in Fe and Ni. Relationships between grain boundary chemistry, electrochemical potential and fracture in aqueous solutions such as fracture mode changes and crack growth rates as a function of grain boundary chemistry and electrochemical potential. Effect of plastic strain and various gaseous environments on the quantity and distribution of surface adsorption will be studied in an Auger electron spectrometer using an in-situ straining stage.

217. SPUTTER-DEPOSITED SUPERCONDUCTORS — $130,000 — 01-3
S. D. Dahlgren, R. Wang, M. T. Thomas

Study of sputter-deposited superconductors; cathodic sputtering; synthesis of new superconducting materials; relation of sputter-deposition parameters to properties; structure and stability of sputter deposits; atomic volume; heats of transformation; relation of critical current and flux pinning force to grain size; role of additives such as oxygen; high-field A-15 compounds; Nb_3Al, $Nb_3(Al\text{-}Ge)$, Nb_3Ge, Nb_3Sn, Nb_3Si; effect of substrate on sputter-deposited superconductor properties; studies of deposit-substrate interfaces using Auger Electron Spectroscopy; surface mapping and depth profiling of chemical segregation for oxidized samples; initial studies of diffusion in sulfur-containing oxide coatings and in silicate glasses. Program to be completed in FY 1979.

218. OXIDATION-, CORROSION- AND WEAR-RESISTANT FINE-GRAINED MATERIALS — $150,000 — 01-3
M. D. Merz, J. T. Prater

Mechanisms of oxidation, corrosion and wear in fine-grained and amorphous materials; relation of properties to structure and microstructure; high temperature oxidation of sputter-deposited stainless steels; Ni-Cr and Ni-Cr alloys with oxide dispersants; diffusion of protective oxide-forming elements; activation energies and rate controlling steps for oxide formation; stress in oxide films; sulfidation resistance; aqueous corrosion of amorphous stainless steel; wear behavior of fine-grained and amorphous materials: $Co_{67}Mo_{19}Si_{10}Cr_3$, $Fe_{80}B_{20}$, Cu and Ni; extremely hard alloys and intermetallic components; diskrider method of wear evaluation in vacuum and controlled atmospheres; coefficient of friction.

PACIFIC NORTHWEST LABORATORY (continued)

219. RADIATION EFFECTS ON METALS — $430,000 — 01-4
J. L. Brimhall, E. P. Simonen, H. E. Kissinger, P. L. Hendrick, L. A. Charlot, E. R. Bradley

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

220. RADIATION DAMAGE IN CERAMICS — $95,000 — 01-4
W. J. Weber, R. P. Turcotte

Particle-induced radiation damage in cubic oxides (fluorite and spinel structures), SiO_2, and rare-earth silicates (apatite structure). Alpha bombardment using actinide sources and alpha-recoil damage in actinide-doped compounds. Structural changes by x-ray diffraction, density, and scanning electron microscopy; damage ingrowth and annealing kinetics. Inert gas diffusion/defect interactions in glass.

221. SPUTTERING PARAMETER INFLUENCES ON MATERIALS STRUCTURE AND BEHAVIOR — $160,000 — 01-5
J. W. Patten, M. A. Bayne

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 include: stoichiometry, structure, properties, and adherence to metallic substrates. Sputtering parameters to be studied include: deposition rate, substrate temperature, bias, and oxygen partial pressure.

PACIFIC NORTHWEST LABORATORY (continued)

222. OPTICAL AND LASER MATERIAL STUDY — $110,000 — 02-2
J. S. Hartman, R. L. Gordon, D. L. Lessor

Examination of optical scattering by controllably roughened metal surfaces; preparation of controllably roughened single crystal copper surfaces; etch pits in copper crystal surfaces; chemical crystal polishing; development of reflective Nomarski microscopy for quantitative surface topography evaluation; development of a detailed optical model for Nomarski reflection microscope; nondestructive, noncontact evaluation of sample surface topography; fractional wavelength vertical topography resolution; particle radiation effect on the optical properties of metal reflectors; copper ion beam incident on copper reflectors; in-situ optical evaluation during irradiation using ellipsometry; ellipsometric examination of surface layers; single crystal copper reflectors; laser fusion reflectors.

223. SPUTTER-DEPOSITED COATINGS FOR OPTICAL APPLICATIONS — $100,000 — 02-2
W. T. Pawlewicz, P. M. Martin, N. Laegreid

Relation of optical properties to structure and stoichiometry; control of structure and stoichiometry through understanding reactive sputtering process; oxides of Ti, Zr, Ta, Nb, Si and In/Sn; refractive index, absorption coefficient and optical band edge by transmission/reflection spectrophotometry; x-ray diffraction, transmission electron microscopy.

224. NANOMETRE MACHINING AND GRINDING DEVELOPMENT — $60,000 — 02-5
D. M. Miller, N. Laegreid

Development of machining and grinding technology permitting achievement of surface roughness less than 1.5 nanometre rms, and total contour accuracy of 100 nanometre for flat, concave and convex spherical and aspherical surfaces up to one metre diameter. The immediate objective is to complete the development of the Omega-X Nanometre Machining System as well as identifying cutting tool, materials and part geometry limitations. The longer term objective is to develop the grinding capability for hard and brittle materials.

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

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

225. 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 variable Cl^- concentration (activity). Austenitic nitronic steels crack in pure anhydrous melts, i.e. with no hydrogen. Cracking behavior with added HCl to be determined. Electrochemical studies to identify reactions which occur during crack extension. Investigation of transient corrosion processes by Digital Faradaic Impedance Measurements and other techniques.

226. ION IMPLANTATION AND DEFECTS IN MATERIALS — $330,000 — 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

Ion beam modification and analysis of near surface regions of solids. Laser annealing of implanted and amorphous solids, H concentration measurements and bonding studies in crystalline and amorphous Si, EPR and optical investigation of defects in laser annealed semiconductors. Ion implantation metallurgy: formation of equilibrium and nonequilibrium alloys, electron beam and laser annealing of ion implanted metals, measurement of diffusion coefficients, solubility, enthalpy and entropy of reaction, phase diagram determinations. Observations of solute trapping, TEM diffraction and microscopy, temper embrittlement of Fe alloys.

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

Basic studies on the erosion and wear of surfaces by abrasion and particulate impact in varying thermal and chemical environments. Effect of chemical environment on the fracture of brittle materials (Rebinder effect) under well-controlled environments, as determined using acoustic emission and other techniques. Substrate-coating interactions in the formation of adherent wear- and erosion-resistant coatings for energy applications. Failure analysis of eroded surfaces and modeling of the erosion mechanisms.

SANDIA LABORATORIES (continued)

228. SEMICONDUCTORS FOR USE AT HIGH TEMPERATURE 01-5

W. V. McLevige C. E. Barnes
L. R. Dawson G. C. Osbourn

In-depth experimental and theoretical studies of defect behavior in compound semiconductors such as GaP, AlGaAs, and GaAs. Defects and their behavior, either thermal or athermal, will be characterized by a variety of techniques including deep level spectroscopy, luminescence and electrical measurements on homojunctions, heterojunctions and metal contacts. Emphasis will be on defects in device-like structures as most of the defects of interest are generated at interfaces between dissimilar materials and because defect behavior is strongly influenced by mechanical stresses at the interfaces and by electrical current (athermal) effects. (Work to be started in FY80.)

SANDIA LABORATORIES (continued)

229. SURFACE PHYSICS RESEARCH $195,000 02-2
J. E. Houston D. R. Jennison
J. A. Panitz R. R. Rye

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. In addition, experimental and theoretical procedures are being developed for retrieving information on the local chemical environment of various adsorbate atoms on solid surfaces using electron spectroscopic techniques. Utilizing gas-phase molecular species as "absolute" standards, Auger Electron Spectroscopy has been demonstrated to be extremely sensitive to detailed chemical environment, and theoretical procedures have been developed which are capable of adequately characterizing the spectroscopic results in terms of local electronic properties.

230. DEVELOPMENT OF A FIELD-DESORPTION MICROSCOPE FOR SURFACE IMAGING $130,000 02-5
J. A. Panitz

An instrument is being developed which utilizes field-desorption techniques to obtain images of 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.

231. HYDROGEN PRODUCTION BY SOLAR PHOTO-ASSISTED ELECTROLYTIC DECOMPOSITION OF WATER $145,000 02-2
M. A. Butler D. S. Ginley
M. L. Knotek B. Morosin
J. E. Schirber

The basic mechanisms of photocatalytic and photosynthetic reactions at semiconductor-electrolyte interfaces are being investigated with emphasis on H production by electrolysis of H_2O. The role of semiconductor electrode properties in determining reaction efficiences and electrode stability are being explored both experimentally and theoretically. Optical and electrochemical spectroscopic techniques are used to delineate the microscopic details of the reaction processes at the semiconductor-electrolyte interface.

SANDIA LABORATORIES (continued)

232. STUDIES OF THE VAPOR PHASE OF THE CHEMICAL-VAPOR-DEPOSITION PROCESS — $120,000 — 02-5

G. H. Miller, A. W. Johnson, P. J. Hargis, M. E. Coltrin

Studies of important vapor-phase reactions and 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 predictive model and improved CVD processing techniques.

233. ELECTRON-STIMULATED DESORPTION: STUDY OF IONICALLY BONDED SURFACES — 02-2

M. L. Knotek, P. J. Feibelman, J. E. Schirber

Study of reactions of H_2O, O_2 and other adsorbates with transition metal oxide surfaces will be performed using the electron stimulated desorption (ESD) technique. The studies will exploit the recent discovery that ESD often occurs through Auger decay of a core hole. High energy thresholds in ESD allow the study of surface bonding in cases where other surface techniques are silent. ESD is atom specific, sensitive to valence and sensitive to the outermost surface layer. To start in FY 1980.

SANDIA LABORATORIES
Livermore, California 94550

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

234. GASES IN METALS $160,000 01-2
W. D. Wilson G. J. Thomas
W. A. Swansiger M. I. Baskes
S. H. Goods C. F. Melius

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.

SOLAR ENERGY RESEARCH INSTITUTE
Golden, Colorado 80401
B. L. Butler - Phone: (FTS) 327-1104 or (303) 231-1104

235. SILVER MIRROR DEGRADATION RESEARCH $200,000 01-1
A. W. Czanderna

To develop an understanding of the physical and chemical changes of silver and silver alloy mirror systems that produce a degradation of the integrated reflectance of incident solar energy; effects of environmental gases and impurities on the stability or reactivity of silver/polymer, silver/glass, and silver/copper interfaces; optical properties and corrosion resistance of silver and silver alloys with Al, Cu, and Be; optical, microgravimetric surface analysis, scanning electron microscopy, ac corrosion, infra-red measurements.

SECTION B

Universities

The information was taken from current 200-Word Summaries provided by the contractor. There is considerable (about 10%) turnover in the University 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.

UNIVERSITY OF ARIZONA

302. CHEMICAL VAPOR DEPOSITION OF AMORPHOUS SILICON FOR PHOTOTHERMAL SOLAR ENERGY CONVERTERS — $120,000 — 02-2
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 photothermal converter stacks operating at temperatures above 550°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

303. INFRARED ABSORPTION SPECTRUM OF FREE CARRIERS IN POLAR SEMICONDUCTORS — $ 40,026 — 02-3
B. Jensen - Dept. of Physics
Phone: (617)-353-2610

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

BROWN UNIVERSITY

304. A COMBINED MACROSCOPIC AND MICROSCOPIC APPROACH TO THE FRACTURE OF METALS — $131,400 — 01-2

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

Correlation of macroscopic fracture mechanics with microstructurally associated deformation and failure mechanisms in metals, mostly steels; correlation with both diffusive and plastic flows; shear localization; numerical analysis of stable crack growth under small scale yielding; correlations and comparison with tearing modulus values; void formation and linkage at grain boundaries and enhancement by H environments.

CALIFORNIA INSTITUTE OF TECHNOLOGY

305. A STUDY OF METAL HYDRIDES AND IONIC CONDUCTORS WITH NUCLEAR MAGNETIC RESONANCE TECHNIQUES — $ 75,000 — 03-1

S. I. Chan, R. W. Vaughan(deceased) -
Chemistry and Chemical Engineering Department
Phone: (213)-795-6811, X2508

Multiple-pulse nuclear magnetic resonance studies of chemical and electronic features of bonds in binary metal hydrides, and the characterization of solid materials showing rapid ion transport at low temperatures. Development of double resonance interferometric examination of ^{23}Na, ^{7}Li, ^{11}B, or ^{27}Al, with applications to beta- and beta"-aluminas (both single-crystal and polycrystal-line) as a function of temperature and ion exchange.

306. THE PRESSURE DEPENDENCE OF THE MECHANICAL PROPERTIES OF POLYMERS — $ 70,000 — 01-2

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

Evaluation of time-temperature-pressure superposition in elastomers; measurement of time-dependent Poisson ratio, shear relaxation modulus, thermal expansivity and compressibility up to 10 kbars; analysis of behavior near glass-transition pressure.

UNIVERSITY OF CALIFORNIA/SAN DIEGO

307. THE RESPONSE OF SUPERCONDUCTORS TO VARIATIONS IN IMPURITY CONTENT AND APPLIED PRESSURE — $204,229 — 02-2

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

This is an experimental research program to investigate the coexistence of superconductivity and magnetism. The primary interest is in A-15's ternary molybdenum chalcogenides, and other high T_c superconductors. Properties of new rare earth compounds such as $ErRh_4B_4$ and $ErMo_6Se_8$ will be studied in order to understand re-entrant and coexistence phenomena. A new effort in surface physics has been started with a study of the oscillatory oxidation of CO on Pt and a study of some metallic thin film oxidations.

308. RESEARCH ON THERMOPHYSICAL PROPERTIES OF MATERIALS — $259,440 — 02-5

J. C. Wheatley - Dept. of Physics
Phone: (714)-452-2490

This is a study of the properties of liquids of one or more components at densities in excess of critical density and under highly nonuniform conditions of temperature using the classical components of Malone's liquid engine as a unique laboratory. Equilibrium thermodynamic data will also be obtained as needed. The first liquids to be worked with are Freon 114, Freon 113, and water. Additionally, we propose to study the effect of electric fields on heat transfer in liquids near their critical points, with first application to Freon 13 and Freon 13B1, and the electrocaloric effect in lead (lanthanum) zirconate titanate with emphasis on its possible application in heat engines. Possible experiments related to the ferromagnetism of superfluid ^3He are also proposed.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA

309. RESONANCE STUDIES OF SUPERIONIC CONDUCTORS — $ 78,378 — 02-2

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 requency 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.

UNIVERSITY OF CALIFORNIA/DAVIS

310. RADIATION DAMAGE AND ENVIRONMENTAL EFFECTS IN HIGH LEVEL WASTE STORAGE GLASSES USING TRANSMISSION ELECTRON MICROSCOPY — $ 64,000 — 01-1

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

The response of H. L. W. S. G. (high level waste storage glasses) to irradiation will be 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. The effects of microstructural features including phase separation, precipitation, devitrification, particle size, and composite annealing temperatures on the properties of H. L. W. S. G. will be investigated. Experimental efforts will involve transmission, high voltage, and analytical electron microscopy, alpha, neutron, electron, and heavy ion irradiation, and leaching experiments.

311. DEFORMATION AND FAILURE MODES IN SUPERPLASTICITY — $ 52,400 — 01-2

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

Experimental study of superplasticity and its relation to creep deformation and rupture; effects of prior cold work and impurity segregation on creep parameters and cavitation in Al-Zn, Cu- and Zr-base alloys.

UNIVERSITY OF CALIFORNIA/IRVINE

312. THE INTERACTION OF LOW ENERGY ELECTRONS WITH SURFACE LATTICE VIBRATIONS — $ 28,751 — 02-3

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

This is a program in theoretical solid state physics which is unique in that it is part of a two proposal program from Professor Doug Mills of the University of California, Irvine, and Professor S. Y. Tong of the University of Wisconsin, Milwaukee. The two PI's recently began a collaboration in the area of inelastic electron scattering from surfaces.

Their intent is to formulate a theory in a modern realistic way so that recent experimental results in high resolution electron energy loss spectroscopy (EELS) can be utilized to full advantage. In these experiments high resolution (8-10 meV) energy analysis of beams both on and off the specular direction allow the vibrational frequencies of clean surfaces as well as adsorbed molecules to be studied in more detail than ever before.

UNIVERSITY OF CALIFORNIA/LOS ANGELES

313. IRRADIATION INDUCED PRECIPITATION IN PALLADIUM-BASE ALLOYS — $ 82,000 — 01-4

A. J. Ardell - Dept. of Materials
Phone: (213)-825-5135

Experimental study of irradiation-induced precipitation in binary Pd-base Ag, Cu, Ni, Mo, W, Ta, Nb, Fe alloys and Ni-Si alloys; 400-1000°C; proton, electron, and heavy-ion irradiations; TEM and AES; effects of solute size-misfit, dose rate, and precipitate stability; relationship between irradiation-induced precipitates and void swelling.

CARNEGIE-MELLON UNIVERSITY

314. FUNDAMENTAL STUDIES OF EROSION AND EROSION/CORROSION FOR COAL GASIFICATION SYSTEMS — $ 57,600 — 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

Modelling 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.

CARNEGIE-MELLON UNIVERSITY

315. KINETICS, MORPHOLOGY AND THERMODYNAMICS OF THE SOLID-LIQUID TRANSITION OF NON-METALS — $ 44,740 — 01-1

R. F. Sekerka - Dept. of Metallurgy and Materials Science
Phone: (412)-621-2600

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.

CASE WESTERN RESERVE UNIVERSITY

316. EXPERIMENTS IN HIGH VOLTAGE AND ANALYTICAL ELECTRON MICROSCOPY — $110,000 — 01-4

T. E. Mitchell and 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, $Y_3Al_5O_{12}$, and Si_3N_4 which are notably resistant to swelling.

317. ENVIRONMENTAL REACTIONS AND THEIR EFFECTS ON MECHANICAL BEHAVIOR OF METALLIC MATERIALS — $ 65,800 — 01-2

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

Experimental investigation of the effects of ion-implanted surface films on dislocation motion and stress-strain behavior of Group VB refractory metals - Nb, Ta at low temperatures; hydride spacing and coherency effects on low temperature deformation of Nb-H; in-situ HVEM straining of ferritic steels in vacuum and low pressures of H.

CASE WESTERN RESERVE UNIVERSITY (Continued)

318. PLASTIC DEFORMATION IN OXIDE CERAMICS — $ 71,200 — 01-2
A. H. Heuer - Dept. of Metallurgical and Materials Sciences
Phone: (216)-368-4224

Plastic deformation of single crystal oxide ceramics at elevated temperatures. Transmission electron microscopy to study dislocation motion and interactions with other crystalline defects, and the correlation with macroscopic stress-strain parameters. Effects of deviations from stoichiometry with its resulting defect structures on dislocation structure and motion. Materials which exhibit different mechanisms of accommodation to nonstoichiometry are presently under study: UO_2, TiO_2, and $MgAl_2O_4$. Annealing kinetics of dislocation loops are studied to determine diffusion kinetics and effects of nonstoichiometry.

319. STUDY OF COUPLED DIFFUSION PHENOMENA IN MULTICOMPONENT GLASSES AND GLASS FORMING LIQUIDS — $ 75,600 — 01-3
A. R. Cooper - Dept. of Metallurgical and Materials Sciences
Phone: (216)-368-4224

Multicomponent diffusional mass transport in both temperature and concentration gradients; theoretical and experimental; chemical potentials and activities; intrinsic and chemical diffusion coefficients; glasses and glass forming liquids; $K_2O{\cdot}SrO{\cdot}SiO_2$ system; microprobe analysis; theory of continuous glassmaking.

CATHOLIC UNIVERSITY OF AMERICA

320. IONIC TRANSPORT AND ELECTRICAL RELAXATION IN GLASS — $ 51,750 — 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

321. FLUX PINNING AND FLUX FLOW STUDIES IN SUPERCONDUCTORS USING FLUX FLOW NOISE TECHNIQUES — $ 55,000 — 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 will be prepared containing various metallurgical defects and exhibiting different critical current characteristics resulting from the defect structure and the flux flow noise power spectrum will be 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.

322. RADIATION EFFECTS IN BCC REFRACTORY METALS AND ALLOYS — $ 31,000 — 01-4

J. Moteff - Dept. of Materials Science and Metallurgical Engineering
Phone: (513)-475-3096

Measurement of hot hardness, creep and tensile behavior, dislocation substructure, void swelling, and cluster formation in neutron-irradiated and irradiated Mo; effect of impurities, temperature and fluence on defect structure and mechanical properties; dispersed barrier model.

COLORADO ENERGY RESEARCH INSTITUTE

323. HYDROGEN AND METHANE SYNTHESES THROUGH RADIATION CATALYSIS — $ 98,191 — 02-2

J. DuBow - Dept. of Electrical Engineering, Colorado State Univ.
Phone: (303)-491-8235

The studies of this research is centered upon hydrogen and methane synthesis through radiation-induced catalysis. The research includes (a) examination of energy transfer mechanisms from characterized catalysts and adsorbed reactants in ionizing radiation environments, (b) doping and tailoring of semiconductor catalysts, and (c) quantitative measurements of radiation-enhanced catalytic reactions.

CALIFORNIA INSTITUTE OF TECHNOLOGY

324. STUDIES OF ALLOY STRUCTURES AND PROPERTIES — $155,000 — 01-1

W. L. Johnson - Division of Engineering
Phone: (213)-795-6811, X1435

Research on the properties and structure of amorphous magnetic or superconducting alloys; ternary amorphous alloys covering the range from ferromagnetism to superconductivity; flux pinning by crystalline phase precipitates embedded in an amorphous superconducting matrix; Fe-P-B amorphous alloys; high temperature amorphous superconductors based on Zr, Mo or Nb; amorphous Gd-La-Au alloys; low temperature specific heat measurements; superconducting tunneling experiments; NMR; Mossbauer techniques used in study of ductile-brittle behavior of amorphous alloys; properties of the mixed state.

COLORADO SCHOOL OF MINES

325. FERROUS ALLOY METALLURGY - LIQUID LITHIUM CORROSION AND WELDING — $100,476 — 01-1

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

Weight loss measurements as a function of temperature and nitrogen content of stainless steel in liquid lithium; grain boundary penetration of stainless steel by liquid lithium; effects of fatigue and creep on corrosion; mechanical testing system capable of a range of tensile, creep and fatigue tests in a liquid metal environment; role of alloying elements in controlling weld metal microstructure in dissimilar metal joints; welding of 2¼ Cr-1 Mo to stainless steel; predictive diagrams for weld structure; role of and analysis for ferrite in welds using Mossbauer techniques and x-ray diffraction.

UNIVERSITY OF COLORADO

326. CRITICAL SCATTERING OF LASER LIGHT BY BULK FLUIDS AND THIN FILMS — $ 85,000 — 02-2

R. Mockler - Dept. of Physics & Astronomy
Phone: (303)-492-7777
W. O'Sullivan - Dept. of Physics & Astronomy
Phone: (303)-492-7457

The dependence upon film thickness of the critical temperature of binary fluid films will be studied using index of refraction techniques. The recently discovered 2-d Ising model scaling behavior will be exploited. The cross-over from three-dimensional Ising model to two dimensional will be studied. In particular Brownian motion in critical fluid films will be observed as the film crosses over to two dimensions.

COLUMBIA UNIVERSITY

327. DEFECT INTERACTIONS AT HIGH CONCENTRATIONS IN SOLID-OXIDE ELECTROLYTES — $ 46,300 — 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 trivalent elements (Y, Gd, La, Sc) of different ionic radius; 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.

328. HIGH TEMPERATURE PROPERTIES OF NUCLEAR REACTOR COOLANTS AND THERMODYNAMIC POWER CYCLE WORKING FLUIDS — $ 47,000 — 03-2
C. F. Bonilla - Dept. of Chemical Engineering
Phone: (212)-280-4441

Determination of the isothermal compressibility of liquid sodium to 3000°F and to measure the vapor pressure of lithium in the critical regime. Surface tension properties of lithium and PVT data for cesium near the critical point.

UNIVERSITY OF CONNECTICUT

329. ELECTRODE POLARIZATION STUDIES IN HOT CORROSION SYSTEMS — $ 49,700 — 01-3
O. F. Devereux - Dept. of Metallurgy
Phone: (203)-486-4714

Electrode polarization studies of metals (Fe, Ni, and steels) in molten carbonate salts containing various H:S:O potentials; determination of electrode reactions and their kinetics and energetics; thermodynamic analysis of Na-salt phase equilibria.

UNIVERSITY OF CONNECTICUT (Continued)

330. ELECTRON-DISLOCATION INTERACTIONS AT LOW TEMPERATURES — $ 54,500 — 01-2
J. M. Galligan - Dept. of Metallurgy
Phone: (203)-486-3541

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

331. MECHANICAL PROPERTIES OF CRYSTALLINE SOLIDS — $ 92,000 — 01-2
Che-Yu Li - Dept. of Materials Science
Phone: (607)-256-4349
E. W. Hart - Dept. of Materials Science
Phone: (607)-2564853

Development of concepts and methods for characterizing mechanical properties of solids based on the state variable approach; TEM measurements of structure data to compare with structure-sensitive parameters; grain boundary anelasticity of nickel by load relaxation and by closed stress-strain loop constant extension-rate testing; grain boundary cavitation of Zircaloy fuel-element cladding; hillock formation in thin films.

332. INELASTIC DEFORMATION IN NON-METALLIC CRYSTALLINE SOLIDS — $ 34,402 — 01-2
D. L. Kohlstedt - Dept. of Materials Science and Engineering
Phone: (607)-256-7144

Inelastic deformation of transition metal carbides with transmission electron microscopy analysis of deformation induced dislocation structures. Constant strain rate, constant stress, and load relaxation experiments; correlation of dislocation substructures to a mechanical equation of state.

CORNELL UNIVERSITY (Continued)

333. DEFECTS IN METAL CRYSTALS — $235,000 — 01-4
D. N. Seidman - Dept. of Materials Science and Engineering
Phone: (607)-256-2365

Field ion microscopy and field ion atom probe techniques used to study vacancies, interstitials, solute atoms, aggregates of point defects such as voids and their interactions with one another; in-situ irradiation; point defect structure of depleted zones in ion-irradiated metals; range profiles of implanted He in W; diffusion behavior of He in Pt; segregation of impurities to voids in neutron irradiated alloys.

334. INFLUENCE OF GRAIN BOUNDARIES ON THE ELECTRICAL TRANSPORT PROPERTIES OF POLYCRYSTALLINE SI FILMS — $ 48,000 — 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 and directionally solidified Si; interactions between lattice dislocations and tilt and twist boundaries; techniques used: transmission electron microscopy, electron beam induced charge in SEM.

335. ENVIRONMENT AND FRACTURE — $ 70,000 — 01-2
H. H. Johnson - Dept. of Materials Sciences and Engineering
Phone: (607)-256-2323

Transient effects and trapping sites associated with H permeation in Fe and steels; trap densities and binding energies in steels; effect of aqueous sulfide environment on H permeation; Nb-H alloy fracture and hydride formation during thermal cycling.

336. MECHANICAL BEHAVIOR OF MATERIALS AND STRUCTURAL ELEMENTS AT ELEVATED TEMPERATURES — $ 82,000 — 01-2
R. H. Lance - Dept. of Theoretical and Applied Mechanics
Phone: (607)-256-4326
E. W. Hart - Dept. of Theoretical and Applied Mechanics
Phone: (607)-4853

Application of constitutive equations to the prediction of deformation behavior of engineering structural elements under various conditions of load and temperature; response to thermal transients in cylindrical and spherical geometries; inelastic bending of beams, thick-walled pipes under torsional loading; boundary element method (BEM) applied to bodies with irregular boundaries and containing stationary cracks.

CORNELL UNIVERSITY (Continued)

337. PROBABILISTIC MODELS OF THE STRESS-RUPTURE OF COMPOSITE MATERIALS — $ 70,000 — 01-2
S. L. Phoenix - Sibley School of Mechanical and Aerospace Engineering
Phone: (607)-256-3462

Development of probabilistic models of tensile strength and stress-rupture of fiber reinforced polymer composites; local vs equal load sharing rules; bounds on number of adjacent fiber breaks initiating failure of very large composite sections.

338. HIGH TEMPERATURE MECHANICAL BEHAVIOR OF SILICON NITRIDE — $ 62,500 — 01-2
R. Raj - Dept. of Materials Science and Engineering
Phone: (607)-256-4040

Mechanisms by which a minority glass phase in the grain boundaries influences the elevated temperature mechanical behavior of ceramics. Kinetics of dissolution/precipitation of β Si_3N_4 from the glass phase; micro-mechanical modelling for slow crack growth; internal fraction; TEM analysis. Slow crack growth in hot pressed Si_3N_4.

339. INITIAL STAGES OF OXIDATION OF METALS — $100,800 — 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.

DARTMOUTH COLLEGE

340. SUPERCONDUCTIVITY IN FILAMENTARY EUTECTIC COMPOSITES — $ 40,535 — 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.

UNIVERSITY OF DELAWARE

341. ANALYSES OF FAILURE MODES IN SHORT FIBER REINFORCED THERMOPLASTICS — $ 31,000 — 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.

DREXEL UNIVERSITY

342. STRAIN HARDENING AND DUCTILITY OF IRON: AXISYMMETRIC VS. PLANE STRAIN ELONGATION — $ 43,700 — 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 SUPERCONDUCTING V_3Si, Nb_3Ge and Nb — $ 63,750 — 02-2

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

Far infrared absorption spectroscopy is used to probe the energy gap ($2\Delta/kT_c$) at the Fermi Surface of the conduction electron distribution in the above mentioned materials. Measurements of the so called transport electron-phonon spectral function $\alpha^2_{tr}F(\omega)$ are also planned. The experiments use a unique FIR laser spectrometer and a conventional Fourier transform FIR spectrometer.

UNIVERSITY OF FLORIDA

344. SYNTHESIS AND CHARACTERIZATION OF NOVEL POLYMERS FROM NON-PETROLEUM SOURCES — $ 84,000 — 03-3

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

The synthesis and characterization of novel polymers for evaluation in the enhanced oil recovery program. "Tailor-made" polymers designed to overcome deficiencies of polymers presently being used, and made from non-petroleum sources such as naturally occurring carbohydrates, proteins, lignins, or polyisoprenes.

345. DEFORMATION PROCESSES IN REFRACTORY METALS — $ 48,100 — 01-2

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

Effect of impurity interstitials (O, H) on dynamic strain aging of refractory metals (Nb, V) and correlation with slow strain rate embrittlement; effect of interstitial clustering; techniques used: internal friction, tensile testing.

GENERAL ELECTRIC CORPORATE RESEARCH AND DEVELOPMENT

346. LOCAL ATOMIC AND ELECTRONIC STRUCTURE IN GLASSY METALLIC ALLOYS — $ 96,438 — 02-2

Ralph E. Carter - 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 method known as EXAFS (extended x-ray absorption fine structure) will be used in conjunction with the Stanford Synchrotron Radiation Lab (SSRL) to study the local atomic distribution in glassy metallic alloys containing Fe, Ni, B, and P. The theory meanwhile will use the resulting atomic structure data as input to cluster calculations employing modern computational techniques from which electronic structure data such as density of states (DOS) and magnetic properties can be inferred.

GENERAL ELECTRIC CORPORATE RESEARCH AND DEVELOPMENT

347. 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

348. INVESTIGATIONS OF INTERMETALLIC ALLOY HYDRIDING MECHANISMS — $ 86,000 — 01-1
B. R. Livesay - Applied Sciences Laboratory
Phone: (404)-894-3489

Mechanism and kinetics of hydriding and dehydriding of $LaNi_5$, $SmCo_5$, and similar hydrogen storage materials; spontaneous magnetization using an in situ automatic torque magnetometer; in situ high pressure microbalance; microscopy including HVEM; micromechanics of decrepitation; pressure-composition isotherms.

349. THE STRUCTURE AND REACTIVITY OF HETEROGENEOUS SURFACES AND STUDIES OF THE GEOMETRY OF SURFACE COMPLEXES — $121,462 — 02-3
U. Landman - Dept. of Physics
Phone: (404)-894-3368

An investigation of methods for the study of the geometry and dynamics of adsorbates 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.

UNIVERSITY OF HOUSTON

350. MICROSTRUCTURAL STUDIES OF HYDROGEN AND OTHER INTERSTITIAL DEFECTS IN BCC REFRACTORY METALS — $ 80,000 — 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 modifications.

ILLINOIS INSTITUTE OF TECHNOLOGY

351. DIFFUSION MECHANISMS AND DEGRADATION OF ENVIRONMENTALLY SENSITIVE COMPOSITE MATERIALS — $ 48,900 — 01-2

L. J. Broutman - Dept. of Metallurgy and Materials Engineering
Phone: (312)-567-3049

Moisture permeation in graphite fiber reinforced epoxy composites and effect on composite strength and failure modes; comparison with changes in degree of cross-linking in epoxy matrix and applied stress during permeation.

352. ELECTROCHEMISTRY OF ACETYLIDES, NITRIDES AND CARBON CATHODES IN MOLTEN HALIDES — $ 52,000 — 03-3

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

Investigation of the electrochemical properties of carbon as a cathode in molten halides, and of the stable acetylides and nitrides of lithium and calcium in molten-halide solutions. Chronopotentiometric and potentiodynamic techniques used for electrode-kinetic studies, and x-ray and ion microscopy techniques used for characterization of carbon substrates and deposits.

JOHNS HOPKINS UNIVERSITY

353. CONDENSATION PROCESSES IN COAL COMBUSTION PRODUCTS — $ 46,000 — 03-3

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

Theoretical and experimental studies of non-equilibrium condensation in fossil-fuel combustion processes, with emphasis on slag vapors and catalyst poisoners. Study of thermal and electrical properties of aerosols, and on the kinetics of nucleation and chemical reactions in such materials as SiO_2 or silicates.

LEHIGH UNIVERSITY

354. ANALYTICAL STUDY OF DRAWING AND EXTRUSION OF SUPERCONDUCTING FILAMENTARY WIRE: FRACTURE PROBLEMS AND EVALUATION OF TEMPERATURE RISE — $ 75,000 — 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 and experimental investigation of extrusion and drawing of multifilamentary superconducting wire; center burst initiation sites; distribution of temperature in workpiece.

355. PRESSURE SINTERING AND CREEP DEFORMATION - A JOINT MODELING APPROACH — $ 52,100 — 01-1

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

Intermediate and final stage hot pressing of polycrystalline ceramics and correlation of resultant densification behavior with creep deformation data. Experimental variables include stress, temperature, oxygen pressure, grain size, and density. Construction of densification and deformation maps. Use of penetration porisometry and quantitative metallography to characterize porosity parameters. STEM microanalytical techniques, lattice-imaging microscopy, and Auger electron microscopy to characterize microchemistry and microstructure. Effects of Ni in Al_2O_3 and effects of Al, Mg, Ca, Zn, and Ti in NiO.

LOUISIANA STATE UNIVERSITY

356. INTER-SUBBAND OPTICAL ABSORPTION IN AN INVERSION LAYER ON A SEMICONDUCTOR SURFACE IN TILTED MAGNETIC FIELDS — $ 31,081 — 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. A semiclassical approximation will be used to gain insight into the system followed by accurate numerical variational calculations.

UNIVERSITY OF MAINE

357. 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

358. ADSORPTION ON METAL SURFACES — $140,136 — 02-2

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

This is a joint theoretical-experimental investigation of certain interactions on surfaces which, although weak compared to typical chemisorption binding energies, are all important in the study of surface reactivity. One in particular is the weak adsorbate-surface interaction involved in the molecular precursor state which will be probed with modern low temperature high vacuum techniques. The other important interaction to be studied is that between adsorbate molecules which results in the formation of islands of various shapes and sizes.

359. ALLOY STRENGTHENING DUE TO ATOMIC ORDER — $ 55,300 — 01-2

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

Representation of grain boundaries, surfaces and cracks in crystals by dislocation arrays; differential geometry analysis of minimum strain energy configurations; elastic and plastic cracks under monotonic tension, cyclic load-unload, and reversed stress conditions.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

360. LOW TEMPERATURE AND NEUTRON PHYSICS STUDIES — $167,143 — 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.

361. SPECTROSCOPIC INVESTIGATIONS OF SMALL MOLECULE INTERACTIONS ON METAL OXIDE SURFACES — $ 86,000 — 03-1

E. I. Solomon - Dept. of Chemistry
Phone: (617)-253-4508
F. R. McFeely - Dept. of Chemistry
Phone: (617)-253-6106

The study of the surface chemistry of metallic oxide systems of importance as catalysts in industrial processes such as hydrogenation, dehydrogenation and dehydration. Primary emphasis on the interaction of chemically relevant molecules (e.g. H_2, CO, CO_2, CH_4) with ZnO, Al_2O_3, and Cr_2O_3 single crystals, using angle-integrated uv photoemission spectroscopy and high resolution energy loss spectroscopy.

362. MICROMECHANICAL MODELLING OF MICROSTRUCTURAL DAMAGE AT ELEVATED TEMPERATURE DURING CREEP OF SUPERALLOYS FOR ENERGY APPLICATIONS — $140,000 — 01-2

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

Analytical and experimental investigation of creep deformation and cracking in metals -- steels and Ni-base alloys; effects of near-boundary deformation on its sliding and on cavitation; observation of cavities in SEM and correlation with boundary orientation.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

363. HIGH TEMPERATURE PROPERTIES AND PROCESSES IN CERAMICS — $ 127,000 — 01-3

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

364. INFLUENCE OF GASEOUS ENVIRONMENT ON NEAR THRESHOLD, LOW GROWTH RATE FATIGUE CRACK PROPAGATION — $ 56,800 — 01-2

R. O. Ritchie - Dept. of Mechanical Engineering
Phone: (617)-253-2311

Experimental study of crack growth in high strength steels in vacuum and at low H pressure; correlation with stress-strain behavior, prior austenite grain size, martensite structure, and impurity segregation.

365. BASIC RESEARCH IN CRYSTALLINE AND NONCRYSTALLINE CERAMIC SYSTEMS — $468,000 — 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

Electrical conduction mechanism operating in Al_2O_3 at elevated temperatures; electronic and ionic conduction in UO_2; dc conductivity and ionic transference in MgO; sintering of ZnO; sintering maps for MgO and Al_2O_3; activated sintering of CaF_2; ion transport and diffusion in KCl; oxidation kinetics of Fe in MgO; calculations of defects and defect clustering in MgO; effect of dislocations in MgO on the modification of dielectric loss; sintering mechanisms in covalent materials; deformation and sintering mapping of UO_2 low temperature microstructure development of cementitious materials; carbide ceramics survey; ionic thermocurrent of defect complexes in MgO; STEM analysis of grain boundary segregation in MgO.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

366. A BASIC STUDY OF ELECTROSLAG WELDING — $ 94,000 — 01-5

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

Modelling and fabrication of low alloy steel weldments; three dimensional analysis of heat generation and conduction in slag phase, effects of single and multiple electrode geometry, immersion depth in slag, and asymmetrical positioning in the weld gap; experimental assessment of the above.

367. KINETIC PROCESSES AT GRAIN BOUNDARIES — $114,561 — 01-1

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

Experimental investigation of kinetic processes in grain boundaries in metals; atomic transport along grain boundaries; interaction of lattice dislocations with grain boundaries; thin-film specimens containing boundaries of controlled geometry; modeling of the kinetics in terms of the dissociation and glide of appropriate grain boundary dislocation segments in the boundaries; diffusion induced boundary migration; STEM; computer simulation; grain boundary dislocation structures in MgO; diffraction from tilt boundaries in gold.

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

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

Investigate electronic conduction in solid oxide electrolytes; a subgroup of fast ionic conductors in which oxygen diffuses rapidly at elevated temperatures. Parameters controlling nonstoichiometry, impurities and electronic mobility. Pure and doped ThO_2 examined for electronic conductivity, thermoelectric power, and ionic transference number. Microstructural studies of second phases, grain boundary effects and segregation.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

369. PROCESSING STUDIES OF POWDER METALLURGICALLY PRODUCED HIGH TEMPERATURE ALLOYS — $ 46,300 — 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.

370. FUNDAMENTAL INVESTIGATIONS OF THE OXIDATION OF ALLOYS IN MULTICOMPONENT GASEOUS ENVIRONMENTS — $ 93,000 — 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; techniques used -- thermogravimetry, STEM, SAM.

MICHIGAN TECHNOLOGICAL UNIVERSITY

371. 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

Grain boundary segregation in metals and effect on properties; stress corrosion cracking, theory and experiment; Auger electron spectroscopy; sulfur segregation 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 liquid Hg.

UNIVERSITY OF MINNESOTA

372. CORROSION PROCESSES AND ENERGY SYSTEMS — $650,000 — 01-1
R. W. Staehle - Institute of Technology
Phone: (612)-373-2955

Research and technology transfer activities in corrosion; multidisciplinary center for corrosion research on fluid flow effects, inhibitors, water chemistry effects, behavior of ceramic materials, corrosion in liquid metal systems; surface interactions with mechanical properties; protective films on metals; atmospheric corrosion of metals, polymers and glasses; research on concentrated and complex electrolytes; technology transfer through the preparation of movies, handbooks and assessments in specific areas of corrosion.

373. FAR INFRARED AND THERMAL STUDIES ON LOW TEMPERATURE MATERIALS — $ 55,248 — 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.

374. A MICROSTRUCTURAL APPROACH TO FATIGUE CRACK PROCESSES IN POLYCRYSTALLINE BCC MATERIALS — $ 54,100 — 01-2
W. W. Gerberich - Dept. of Chemical Engineering and Materials Science
Phone: (612)-373-4829

Fatigue crack initiation and growth near the threshold in Fe and its binary alloys, steels, and Ti-30 Mo; monotonic and cyclic stress-strain behavior; effects of grain size and precipitates; modeling in terms of dislocation dynamics parameters; techniques used: electron channeling, TEM, SEM.

UNIVERSITY OF MISSOURI

375. ELECTRONIC PROPERTIES OF AMORPHOUS SILICON DIOXIDE AND METALLIC IONS IN SILICATE GLASSES — $ 20,530 — 01-1

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

The electronic properties of crystalline silicon dioxide, amorphous silicon dioxide, and silicate glasses are to be studied by means of a first principle 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.

NEW MEXICO INSTITUTE OF MINING AND TECHNOLOGY

376. CHARACTERIZATION OF EXTRINSIC GRAIN BOUNDARY DISLOCATIONS AND GRAIN BOUNDARY DISLOCATION SOURCES BY TRANSMISSION ELECTRON MICROSCOPY — $ 60,000 — 01-1

L. E. Murr - Dept. of Metallurgical and Materials Engineering
Phone: (505)-835-5011

Characterization of grain boundary ledges and arrays of dislocations at grain boundaries in 304 stainless steel; investigation of ledges as dislocation sources during TEM in situ straining.

377. MICROSTRUCTURAL AND MECHANICAL PROPERTY STUDY OF SOLAR ENERGY COLLECTORS — $ 76,871 — 01-1

O. T. Inal - Dept. of Metallurgical and Materials Engineering
Phone: (505)-835-5011

Effect of plating geometry, bath compositions and current densities on the surface structure of electroplated black chrome; transmission electron microscopy, hardness, solar energy absorption studies; nucleation studies using field ion microscopy; thermal cyclic effects; studies of zinc oxide.

CITY UNIVERSITY OF NEW YORK, CITY COLLEGE

378. MELTING PHENOMENA INVESTIGATED BY LASER LIGHT SCATTERING — $ 67,502 — 02-2
H. Z. Cummins - Dept. of Physics
Phone: (212)-690-6921

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

379. CRITICAL CONDITIONS FOR THE GROWTH OF SiC, Si_3N_4, AND SiO_2 — $ 96,239 — 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 ultra-high 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/BINGHAMTON

380. ENERGIES AND BONDING IN PHOSPHIDES — $ 27,000 — 03-3
C. E. Myers - Dept. of Chemistry
Phone: (607)-798-2269

Systematic interrelations among the atomization enthalpies, electron binding energies, structures, and bonding in manganese phosphides and in other transition metal phosphides. X-ray photoelectron spectroscopy of manganese and iron phosphides; effusion studies on the two-phase regions of the nickel-phosphorus system, and the study of the Mn-P system by high temperature solid state galvanic cells.

STATE UNIVERSITY OF NEW YORK/STONY BROOK

381. THEORETICAL STUDIES OF CHEMISORPTION ON TRANSITION METAL SURFACES: INTERACTION OF HYDROGEN WITH TITANIUM — $ 72,968 — 02-3

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

This research is concerned with the theory of chemisorption of molecules on solid surfaces and is directed toward the development of a theoretical model for treating electronic interactions at an ab-initio level. Calculations on the hydrogen-titanium system are proposed in which the objective is to obtain a detailed account of molecule-surface interactions including an adequate response of the lattice to the adsorbate. The removal of special surface atoms will replicate the formation of a step.

382. PREPARATION, CHARACTERIZATION AND USE OF METAL HYDRIDES FOR FUEL SYSTEMS — $ 53,993 — 01-1

P. J. Herley - Dept. of Materials Science
Phone: (516)-246-6759

Effects of various pretreatments on the thermal decomposition kinetics of aluminum hydride powder; determination of kinetic parameters governing thermal decomposition; effects of gamma-ray pre-irradiation; photo-decomposition with high intensity uv light; activation energies and chemical order of reactions; lithium aluminum hydride, magnesium aluminum hydride, and magnesium hydride; mechanisms underlying decomposition reactions; preparation and recrystallization of high purity hydrides; atomic hydrogen bombardment.

UNIVERSITY OF NORTH CAROLINA

383. THE STRUCTURE OF NEUTRON DAMAGE IN IONIC REFRACTORY OXIDES — $ 37,827 — 01-4

J. H. Crawford, Jr. - Dept. of Physics and Astronomy
Phone: (919)-933-2078

Structure of fast particle induced lattice defects. 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

384. HIGH PRESSURE STUDIES TO DETERMINE THE EFFECTS OF VOLUME AND TEMPERATURE ON THE LATTICE DYNAMICS OF MOLECULAR SOLIDS — $ 39,275 — 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.

385. EQUILIBRIUM AND TRANSPORT PROPERTIES OF DISORDERED TRANSITION AND NOBLE METAL ALLOYS — $ 41,000 — 02-3

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

Theoretical studies of equilibrium and transport properties using the average t-matrix approximately (ATA) applied to a variety of disordered alloys with noble metal base and polyvalent solute.

NORTHWESTERN UNIVERSITY

386. EFFECT OF POINT DEFECTS ON MECHANICAL PROPERTIES OF METALS — $ 90,200 — 01-4

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

Stress-strain behavior of bcc metals Nb and Fe at low temperature; effect of self interstitials from electron radiation, impurities, crystallographic orientation, and surface coatings on dislocation mobility and homogeneous deformation vs. slip band formation; techniques used: HVEM, TEM.

NORTHWESTERN UNIVERSITY (continued

387. INVESTIGATION OF DEEP LEVEL DEFECTS IN EPITAXIAL SEMICONDUCTING ZINC SULPHO-SELENIDE — $ 44,391 — 01-3
B. W. Wessels - Dept. of Materials Science and Engineering
Phone: (312)-492-3536

Preparation of high purity ZnS_xSe_{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 microscopy on deliberately doped n-type and p-type material. Role of misfit dislocations on deep level defects.

388. 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. Experiment techniques include Raman spectroscopy, NMR line-narrowing, and the chemical preparation and crystal growth of selected electrolyte materials.

389. STUDIES OF METAL-SEMICONDUCTOR INTERFACES IN CATALYSIS AND ENERGY CONVERSION — $ 66,000 — 03-1
Y- W. Chung - Dept. of Materials Science and Engineering
Phone: (312)-492-3584

The study of the properties of metal-semiconductor interfaces in nickel methanation and photochemical energy conversion. Emphasis will be on the electronic properties of the interface between nickel and its support (either TiO_2 or ThO_2) and the chemisorption of H_2, CO and H_2S on supported Ni surfaces.

NORTHWESTERN UNIVERSITY (continued)

390. INVESTIGATION OF DISPERSED IRON ALLOY CATALYSTS IN THE CARBON MONOXIDE-HYDROGEN SYNTHESIS REACTION — $ 83,732 — 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

Study of highly dispersed binary iron alloys and their carbides as formed in the CO-H_2 synthesis reaction; iron-copper and iron-alkali systems; determination of particle sizes, shapes and size distribution using Fourier analysis, X-ray line broadening, and transmission electron microscopy; precise determination of the carbide structure using temperature variation in Mossbauer experimental experiments to characterize the magnetic saturation structure; bonding of CO on the exposed metal and carbide surfaces; dispersed metal catalysts prepared by impregnation of metal salts on silica gel, calcination, and subsequent reduction in hydrogen.

UNIVERSITY OF NOTRE DAME

391. PORE SHRINKAGE AND OSTWALD RIPENING IN METALLIC SYSTEMS — $ 60,523 — 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; ripening of pores and voids in sintered compacts of nickel and in nickel 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

392. ELECTRICAL TRANSPORT AND OPTICAL PROPERTIES OF RANDOM SMALL PARTICLE COMPOSITES — $ 93,264 — 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.

393. FUNDAMENTAL STUDIES OF HIGH TEMPERATURE CORROSION REACTIONS — $ 88,500 — 01-3

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

Corrosion of metals in gaseous environments over a range of S:O potentials; mechanisms and kinetics of sulfidation of Mo; scale formation and breakdown; electronic and ionic conduction mechanisms in solid electrolytes; technique used: SEM.

394. HYDROGEN ATTACK OF STEEL — $ 42,465 — 01-2

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

Hydrogen attack kinetics; growth rate of small diameter methane bubbles; rate limiting processes; nucleation site evaluation by SEM with EDAX and scanning Auger; effect of dioxidation practice; determination of carbon activity.

OKLAHOMA STATE UNIVERSITY

395. ELECTRONIC STRUCTURE OF DEFECTS IN OXIDES — $ 27,500 — 02-2

G. P. Summers - Dept. of Physics
Phone: (405) 624-5813

Photoconductivity and fluorescence measurements in oxides -- α-Al_2O_3, CaO, SrO, and spinels; 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.

PENNSYLVANIA STATE UNIVERSITY

396. PHYSICAL ADSORPTION: RARE GAS ATOMS NEAR SOLID SURFACES — $ 18,338 — 02-3
M. W. Cole - Dept. of Physics
Phone: (814) 863-0165

This is a theoretical investigation of the interaction $V(\vec{r})$ between rare gas atoms and crystalline surfaces. Experimental results for specular and diffractive intensities of atomic beam scattering from crystals provide a principal input to the determination of $V(\vec{r})$. Predictions will be made on the basis of realistic and model potentials of the dependence on incident angles and energy of diffractive intensities expected in future measurements. Inelastic scattering will be explored in collaboration with the group performing the experiment. Attention will be focused initially on graphite and alkali halide surfaces, but emerging data for other surfaces will also be studied.

397. HYDROGEN ABSORPTION IN METALS: A FIELD ION MICROSCOPY STUDY — $ 49,500 — 01-1
H. W. Pickering - Department of Materials Sciences and Engineering
Phone: (814) 865-5446
T. Sakurai - Dept. of Physics
Phone: (814) 863-2115

H absorption and trapping in Fe and Ni; effects of impurities and defects on partitioning of H and alloy atom positions; H diffusion; technique used: field ion microscopy.

398. 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
J. W. Halloran - Dept. of Materials Science
Phone: (814) 865-2262

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.

PENNSYLVANIA STATE UNIVERSITY (continued)

399. SUPERPLASTICITY AND FRACTURE OF CERAMICS — $ 38,500 — 01-2
R. C. Bradt - Dept. of Materials Science
Phone: (814) 865-4631

Superplastic deformation during phase transitions and effects of stoichiometry 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_3, MoO_3), where R_2O_3 is a rare earth oxide, with 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 $MgAl_2O_4$. Structural and temperature effects on the fracture process in polycrystalline $MgO \cdot XAl_2O_3$.

400. STRUCTURE OF GLASSES CONTAINING TRANSITION METAL IONS — $ 72,500 — 01-1
W. B. White - Materials Research Laboratory
Phone: (814) 865-1152

Transition metal ion-containing insulator glasses are being studied by Raman, optical absorption, luminescence, and sputter-induced optical emission spectroscopy. Thrusts are (1) structure and phase separation of alkali-alumina-silica and borosilicate glasses, (2) local environment and thermodynamics of Fe, Mn, Ni, and Ti, and (3) dissolution and diffusion processes in glasses.

401. ATOMISTIC STUDIES OF GRAIN BOUNDARIES WITH SEGREGATED IMPURITIES — $ 44,300 — 01-1
V. Vitek - Dept. of Metallurgy and Materials Science
Phone: (215) 243-7883

Computer simulation of grain boundary structure in dilute Au binary alloys; influence of metallic solutes, degree of segregation, and boundary periodicity.

402. ELECTROCHEMICAL INVESTIGATION OF NOVEL ELECTRODE MATERIALS — $ 99,000 — 03-2
W. L. Worrell - Dept. of Metallurgy and Materials Science
Phone: (215) 243-8592

New electrode materials from the dichalcogenides of the Group IV and V transition metals intercalated with lithium and/or sodium. Electrochemical cell techniques to measure chemical potential and diffusion of lithium or sodium with composition x in Li_xMS_2 compounds.

PRINCETON UNIVERSITY

403. CHEMICAL POISONING IN HETEROGENEOUSLY CATALYZED REACTIONS — $ 52,000 — 03-1
S. L. Bernasek - Dept. of Chemistry
Phone: (609) 452-4986

Poisoning by molecules containing Group Vb and VIb atoms (nitrogen and sulfur). Single crystal surfaces of molybdenum and cobalt characterized by LEED and ESCA to examine catalytic activity. Reactions forming formic acid hydrogenation of carbon monoxide and hydrogenolysis of cyclopropane used as model reactions to study poisoning mechanisms and the kinetics of heterogeneously catalyzed reactions.

PURDUE UNIVERSITY

404. HIGH TEMPERATURE EFFECTS OF INTERNAL GAS PRESSURES IN CERAMICS — $ 63,600 — 01-3
A. A. Solomon - Dept. of Nuclear Engineering
Phone: (317) 494-7190

Experimental study of the role of entrapped gases and microstructure on the rate-controlling mechanisms of pressure induced densification and swelling of ceramics; grain size and stoichiometry effects; single and polycrystalline CoO; sintering of CoO; hot pressing and swelling of ZnO; sintering and swelling in carbonyl Ni.

405. STUDY OF ELECTRONS PHOTOEMITTED FROM FIELD EMISSION TIPS — $ 45,763 — 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.

RENSSELAER POLYTECHNIC INSTITUTE

406. PROPERTIES OF GLASS WITH HIGH WATER CONTENT — $ 75,690 — 01-3

M. Tomozawa - Dept. of Materials Engineering
Phone: (518) 270-6451
E. Bruce Watson - Dept. of Geology
Phone: (518) 270-6474

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 650°C. Radiation effects, chemical durability, diffusion, mechanical strength, ion transport processes, differential thermal analysis, thermogravimetric analysis.

407. PROTECTIVE OXIDE FILMS — $ 85,000 — 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.

408. FATIGUE BEHAVIOR OF BCC METALS — $ 46,715 — 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.

RENSSELAER POLYTECHNIC INSTITUTE

409. LOCALIZED CORROSION AND STRESS CORROSION CRACKING BEHAVIOR OF AUSTENITIC STAINLESS STEEL WELDMENTS CONTAINING RETAINED FERRITE — $ 80,000 — 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; pitting corrosion studied at room temperature and 290°C in pressure vessels utilizing potentiodynamic and galvanokinetic test procedures coupled with optical and electron metallography; effect of P and S on pitting corrosion; scanning Auger electron spectroscopy on austenite/ferrite interfaces; slow extension rate stress corrosion cracking experiments; analytical electron microscopy.

410. THERMOPHYSICAL PROPERTIES OF INORGANIC POLYSULFIDES — $ 75,000 — 03-2

G. J. Janz - Dept. of Chemistry
Phone: (518) 270-6344

Synthesis and measurement of thermophysical properties of inorganic polysulfides of importance to advanced electrical storage battery systems.

411. CHEMICAL DIFFUSION ON SOLID SURFACES — $ 34,000 — 01-3

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

Measurement of rates of migration of adsorbed atoms and molecules over solid surfaces; systems studied: H on Ni, Ag on Al_2O_3; techniques used: AES, mass spectrometry.

RICE UNIVERSITY

412. THE EFFECT OF TENSILE BIAS STRESS UPON THE ULTRASONIC ATTENUATION AND VELOCITY OF ULTRA-HIGH PURITY (UNDOPED AND DOPED) TUNGSTEN, MOLYBDENUM, TANTALUM, AND NIOBIUM SINGLE CRYSTALS — $ -0- — 01-2

J. M. Roberts - Dept. of Mechanical Engineering and Materials Science
Phone: (713) 527-3590

Effect of tensile bias stress on ultrasonic attenuation and velocity in pure and doped body centered cubic metallic single crystals; internal friction; physical acoustics; dislocations; flow stress; elastic constants; preparation of high purity bcc metal single crystals.

UNIVERSITY OF ROCHESTER

413. MATERIALS AND MECHANICS OF RATE EFFECTS IN BRITTLE FRACTURE — $ 60,000 — 01-2
S. J. Burns - Dept. of Mechanical and Aerospace Sciences
Phone: (716) 275-4082

Brittle fracture studies using double cantilever beam specimen; crack velocity studies; brittle plastic PMMA, steels and titanium alloys; critical stress intensity factors; crack velocity near the ductile to brittle transition temperature; energy balance analysis; comparison of slow crack velocities, crack extension forces and test temperatures to the theory of thermally activated crack propagation.

414. DIFFUSIONAL CREEP OF MULTI-COMPONENT SYSTEMS — $ 63,000 — 01-2
J. C. M. Li - Dept. of Mechanical and Aerospace Sciences
Phone: (716) 275-4038

Study of diffusion and diffusion related processes such as creep in relatively complex systems; laser-excited diffusion; impression creep; photoelastic studies in epoxy; pencil slip in beta-tin; laser-excited creep in germanium, napthalene and quartz; effect of laser radiation on the ionic conductivity in alkali halide crystals; impression creep of polycrystalline Al and Cu; microimpression elasticity and impression toughness.

ROCKWELL INTERNATIONAL SCIENCE CENTER

415. ACOUSTIC EMISSION SIGNATURE ANALYSIS — $ 91,000 — 01-5
O. Buck - Science Center
Phone: (805) 498-4545

Application of acoustic emission to detection of cracking mechanisms in metals; crack growth in embrittled steels; sustained load cracking of hydrogen embrittled steel; multiple transducer Fourier frequency analysis of acoustic emissions; fracture momentum concept.

ROCKWELL INTERNATIONAL SCIENCE CENTER (continued)

416. SINTERING PHENOMENA OF NON-OXIDE SILICON COMPOUNDS — $ 79,725 — 01-1

D. R. Clarke
Phone: (805) 498-4545
F. F. Lange
Phone: (805) 498-4545

Studies to understand the volatalization 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

417. Solar Energy Research Institute - University Programs
A. Kotch - SERI - Phone: (303) 231-1823

University programs funded through SERI:

University of Nebraska (Eckhardt) $ 40,157
"Optical and Electrical Properties of Organic Dye Crystals"

University of Missouri (Boone/Van Doren) $ 68,638
"Chemical Spray Techniques for Growth of Thin Film CdTe Solar Cell Materials."

Brown University (Gerritsen/Nurmikko) $ 83,730
"Characterization of Photovoltaic Interfaces By Picosecond Optical Methods"

North Carolina State (Hanck/Schreiner/Littlejohn) $74,000
"Electrodeposition of Semiconductors and Photovoltaic Solar Cells"

University of Vermont (Anderson) $ 72,600
"Influence of the Interfacial Layer on Electro-optical Properties of Heterojunction Solar Cells"

University of Florida (Holloway) $ 33,994
"Kinetics and Mechanisms of Degradation of Metal Black Selective Solar Absorber Coatings"

University of Delaware (Fagen) $ 73,300
"Transport Properties of Amorphous Silicon-Germanium Alloy Films"

UNIVERSITY OF SOUTHERN CALIFORNIA

418. ELECTRICAL AND MECHANICAL PROPERTIES OF OXIDE CERAMICS — $ 61,800 — 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 Al_2O_3 with emphasis on the delineation between grain boundary and bulk effects.

419. GRAIN BOUNDARY SLIDING AND DEFORMATION MECHANISMS DURING HIGH TEMPERATURE CREEP — $ 88,000 — 01-2
T. G. Langdon - Dept. of Materials Science and Mechanical Engineering
Phone: (213) 741-2095

Experimental investigation of creep deformation and failure mechanisms in Al- and Mg- base alloys, and ceramics (alkali halides, oxides); measurement of grain boundary sliding and cavitation; TEM characterization of dislocation substructure; effects, of partial unloading; deformation and fracture map construction.

420. EVAPORATION DRIVEN LIQUID SINTERING — $ 43,120 — 01-1
J. W. Whelan - Dept. of Materials Sciences
Phone: (213) 741-6219

Theoretical and experimental studies of the evaporation driven liquid sintering process; vapor transport; effects of particle size, liquid volume fraction, and sintering temperature; density and microstructure as a function of time; MgO-LiF, WC-Cu, and Si_3N_4 with additives.

SOUTHWEST RESEARCH INSTITUTE

421. THE STUDY AND MODELLING OF HIGH TEMPERATURE FATIGUE CRACK PROPAGATION IN AUSTENITIC STAINLESS STEEL — $ 60,184 — 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

422. EXCITED STATE ENERGY TRANSPORT IN SOLUTIONS AND AMORPHOUS MATERIALS — $ 79,000 — 03-1
M. D. Fayer - Dept. of Chemistry
Phone: (415) 497-4446

Theoretical and experimental studies of transport of electronic excitation in disordered systems, using the picosecond transient diffraction grating technique.

423. PHOTOVOLTAIC MATERIALS RESEARCH-II-VI HETEROJUNCTIONS AND Cu_2S/CdS THIN FILMS — $133,000 — 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.

424. MODELING OF DEFORMATION AND FRACTURE IN HIGH-TEMPERATURE STRUCTURAL MATERIALS — $120,000 — 01-2
A. K. Miller - Dept. of Materials Sciences
Phone: (415) 497-3732
O. D. Sherby - Dept. of Materials Sciences
Phone: (415) 497-2536

Use of a computer-based set of constitutive equations for non-elastic deformation, "MATMOD"; solute strengthening in austenitic stainless steel, creep-fatigue interaction in 2 1/4 Cr-1Mo steel; determination of back-stresses and their recovery; strain softening; elevated temperature kinematic hardening; transient subgrain hardening.

STANFORD UNIVERSITY (continued)

425. MECHANISMS AND MECHANICS OF HIGH TEMPERATURE FRACTURE OF MATERIALS — $ 72,800 — 01-2
W. D. Nix - Dept. of Materials Science and Engineering
Phone: (415) 497-4259

Study of creep cavitation and cracking in Ag and Cu with implanted H_2O bubbles; cavity nucleation and growth kinetics and energetics; diffusional flow and creep deformation in fine grained Ni; analyses of grain switching in superplasticity and cavity shape; effect of segregation on creep of steel.

426. DIFFUSION OF OXYGEN IN LIQUID METAL SYSTEMS — $ 53,531 — 01-3
D. A. Stevenson - Dept. of Materials Science and Engineering
Phone: (415) 497-4251

Determination of thermodynamic properties of oxygen in liquid metal solutions using solid state electrochemical techniques. Measurement and interpretation of the chemical diffusion coefficient of oxygen in both pure and alloy liquid metals, thermodynamic activity of oxygen as a function of oxygen composition, saturation concentration of oxygen in liquid metals, Gibbs free energy of formation of respective oxides, thermodynamics of binary liquid metal solutions, and solute interactions in liquid metal solutions. While the effort is primarily experimental, the results are correlated with liquid solution theory.

427. SUPERCONDUCTING AND SEMICONDUCTING PROPERTIES OF ELECTRON BEAM EVAPORATED MATERIALS — $100,000 — 02-2
T. H. Geballe - W. W. Hansen Laboratories of Physics
Phone: (415) 497-4027
M. R. Beasley - W. W. Hansen Laboratories of Physics
Phone: (415) 497-4027

This is research to study the high magnetic field properties of superconducting films prepared using newly developed electron beam coevaporation techniques. The materials to be investigated are A15's such as Nb_3Sn and also ductile alloys. Superconductor parameters as well as strain tolerance, micro-hardness and high temperature mechanical deformation will be studied as a function of composition and microstructure.

SYRACUSE UNIVERSITY

428. SURFACE CHARACTERIZATION OF CATALYTICALLY ACTIVE METAL ALLOY AND COMPOUND FILMS — $106,900 — 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

429. 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

Thermodynamic study of nickel-based alloys; Ni-Mo, Ni-Ta, Ni-Nb, and Ni-W, high-temperature Gibbs free-energy data by a galvanic-cell method; heat capacities of stable and metastable single-phase alloys; thermodynamic functions between 4 and 1400K; computer coupling to obtain integrated thermodynamics and phase diagrams; effect of elastic, vibrational, electronic, and ordering terms.

UNIVERSITY OF UTAH

430. THE EFFECT OF PROCESSING CONDITIONS ON THE RELIABILITY OF CROSS-LINKED POLYETHYLENE CABLE INSULATION — $ 74,000 — 03-2

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

The effect of composition, cross-linking agents and processing on the structure and durability of polyethylene cable insulation under electrical stress.

UNIVERSITY OF UTAH (continued)

431. ELECTROLYTIC DEGRADATION OF LITHIA-STABILIZED β" ALUMINA — $ 68,000 — 03-2
A. V. Virkar - Dept. of Materials Science and Engineering
Phone: (801) 581-5396

Electrolytic degradation from stress corrosion and fracture characterized by current density, composition, and time, for β and β" alumina ceramics immersed in liquid sodium. Surface crack growth and propagation examined and compared with theoretical models.

432. IMPURITY EFFECTS ON THE CREEP OF POLYCRYSTALLINE MAGNESIUM AND ALUMINUM OXIDES AT ELEVATED TEMPERATURES — $ 46,081 — 01-2
R. S. Gordon - Materials Science and Engineering Division
Phone (801) 581-6612

Determination of mechanisms of high temperature creep of polycrystalline oxide ceramics; creep deformation maps; role of aliovalent additives in determining roles of diffusion, grain boundary sliding, and dislocation mechanisms of creep; effects of additives, temperature, oxygen pressure and grain size; MgO and Al_2O_3 doped with Fe, Cr, and Mn-Ti; deformation maps. Experimental activities include creep, stress relaxation creep, and electron spin resonance.

VARIAN ASSOCIATES SOLID STATE LABORATORY

433. RESEARCH ON LATTICE MISMATCHED SEMICONDUCTOR LAYERS — $ 99,876 — 01-3
R. L. Moon
Phone: (415) 493-4000 x3278
R. L. Bell -
Phone: (415) 493-4000 x2906

Morphology and properties of semiconducting III-V compound ternary, quaternary and quinary epitaxial layers grown lattice-mixmatched on substrates with reference to their ultimate applications in high efficiency solar cells; organometallic VPE growth of AlGaAsSb characteristics of materials grown by the liquid phase melt depletion lattice parameter grading method; AlGaAsSb and GsAsP systems; incorporation of high densities of ionizable donor and acceptor species; minority carrier lifetimes and surface recombination; high voltage electron microscopy; X-ray topography; dislocation etch pit analysis; pn junction characteristics and analysis by photoluminescence and spectral response; organometallic vapor phase epitaxy; Hall measurements; AlGaAsSb phase diagram calculations.

VIRGINIA POLYTECHNIC INSTITUTE
AND STATE UNIVERSITY

434. HYDROGEN EMBRITTLEMENT TESTING — $ 33,000 — 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

435. SPECTROSCOPY OF SURFACE ADSORBED MOLECULES — $ 89,623 — 02-2
R. V. Coleman - Dept. of Physics
Phone: (804) 924-3781

Inelastic electron tunneling spectroscopy (IETS) will be used to study the vibrational spectra of molecules adsorbed on oxide surfaces. These measurements are being augmented with PES and AES studies. The latter will provide data on the electronic structure which will help elucidate the vibrational data from IETS.

WASHINGTON UNIVERSITY

436. DETERMINATIONS OF LATTICE AND ELECTRONIC STRUCTURES OF SOLIDS BY ELECTRON SCATTERING — $ 56,146 — 02-2
P. C. Gibbons - Dept. of Physics
Phone: (314) 889-6271

This project will develop and demonstrate methods for determining lattice and electronic structures within a few Angstroms of selected atomic species, with measurements that average over the chosen sites in sample areas less than one micron in diameter. The areal resolution is provided by the electron optics of a conventional transmission electron microscope. Electron energy-loss spectroscopy of core-hole excitations reveals rich structure due to atomic and solid-state effects. The momentum-transfer dependence of the electron scattering spectra allows unique identification of most spectral features, in terms of the physical processes causing them. EXAFS (extended X-ray absorption fine structure) modulation contains lattice information and features near threshold are sensitive to details of the electronic structure. Polycrystalline semiconductors and metals and composite metals will be surveyed to identify promising directions for further study.

UNIVERSITY OF WASHINGTON

437. NUCLEAR MAGNETIC RESONANCE STUDIES OF ION MOTION IN SOLID ELECTROLYTES — $ 46,449 — 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 (1) β-alumina, (2) lithium nitride, and (3) rubidium silver iodide.

COLLEGE OF WILLIAM AND MARY

438. A THEORY OF THE ELECTRONIC PROPERTIES OF SEMICONDUCTOR ALLOYS — $ 53,100 — 02-3

A. Sher - Dept. of Physics
Phone: (804) 253-4471

This is a theoretical proposal aimed at accurate predictions of the electronic behavior of a wide variety of semiconductor alloys. The principal theoretical technique to be used is the coherent potential approximation (CPA) augmented with parameterized band structures of the alloy constituents. This results in a simple enough procedure that a large number and variety of systems can be treated. In addition a great number of properties such as band gap, effective masses, optical spectra, alloy scattering rates and mobility temperature.

UNIVERSITY OF WISCONSIN

439. LOCAL ELECTRONIC PROPERTIES OF SEMICONDUCTOR SURFACES AND INTERFACES — $ 85,000 — 02-2

M. G. Lagally - Dept. of Metallurgical and Mineral Engineering
Phone: (608) 263-2078

The local electronic properties of surfaces and interfaces of some elemental and compound semiconductors, e.g. GeS, GeSe, SnS and SnSe will be studied using Auger Electron Spectroscopy (AES). In addition chemisorption of Cl and O on Si will be investigated. AES will be augmented with XPS and UPS in all of these studies. Electron stimulated disorption methods will also be used. This year SiC, Si_3N_4 and BN will be added to the list of materials studied.

UNIVERSITY OF WISCONSIN (continued)

440. PREDICTION OF THE BEHAVIOR OF STRUCTURAL MATERIALS UNDER IRRADIATION THROUGH MODELLING OF THE MICROSTRUCTURE — $ 20,000 — 01-4
W. G. Wolfer - Dept. of Nuclear Engineering
Phone: (608) 263-6818

Modelling of nucleation and growth of radiation-induced voids and dislocations; effects of spatial correlations between sinks for point defects and of the time dependence of their production; evaluation of irradiation-enhanced creep models---stress-induced preferential absorption (of defects) and climb-controlled glide; crystallographic orientation effects.

441. VOID NUCLEATION AND GROWTH IN HEAVY ION AND ELECTRON BOMBARDED PURE METALS — $ 21,939 — 01-4
G. L. Kulcinski - Dept. of Nuclear Engineering
Phone: (608) 263-2308
P. Wilkes - Dept. of Nuclear Engineering
Phone: (608) 263-2196

Irradiation variables and material parameters influencing void formation and swelling in pure Al, Al alloys, pure V, and V-N alloys. Electrons and heavy ions are being used, the latter to simulate neutron irradiation. The effects of irradiation temperature, fluence, flux, impurities, and annealing on void nucleation and growth are being studied. Precision ($\sim$20Å) length change measurements are used to follow various annealing stages.

UNIVERSITY OF WISCONSIN, MILWAUKEE

442. THE INTERACTION OF LOW ENERGY ELECTRONS WITH SURFACE LATTICE VIBRATIONS — $ 37,675 — 02-3
S. Y. Tong - Dept. of Physics
Phone: (414) 963-4474

This is a program in theoretical solid state physics which is unique in that it is part of a two proposal program from Professor Doug Mills of the University of California, Irvine, and Professor S. Y. Tong of the University of Wisconsin, Milwaukee. The two PI's recently began a collaboration in the area of inelastic electron scattering from surfaces.

Their intent is to formulate a theory in a modern realistic way so that recent experimental results in high resolution electron energy loss spectroscopy (EELS) can be utilized to full advantage. In these experiments high resolution (8-10 meV) energy analysis of beams both on and off the specular direction allow the vibrational frequencies of clean surfaces as well as adsorbed molecules to be studied in more detail than ever before.

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 $68.5 million in operating funds (budget outlays) and $5.9 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.)	42.5	18.0
(b) South ..... (Fla., N.C., Tenn., Va., La., Ga.)	6.2	22.1
(c) Midwest ..... (Ohio, Ill., Wisc., Mich., Mo., Minn., Ind., Iowa, Kan.)	20.7	38.2
(d) West ..... (Ariz., Okla., Wash., Texas, N. Mex., Calif., Utah, Colo., Idaho)	30.6	21.7
	100.0	100.0

2. By Academic Department or Laboratory Division:

	Contract Research (% by $)	Total Program (% by $)
(a) Metallurgy, Materials Science, Ceramics (Office Budget Activity Numbers 01-)	64.2	44.0

	Contract Research (% by $)	Total Program (% by $)
(b) Physics, Solid State Science, Solid State Physics (Office Budget Activity Numbers 02-)	26.1	42.1
(c) Chemistry, Chemical Eng. (Office Budget Activity Numbers 03-)	9.7	13.9
	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)	35.6
(b) DOE Laboratory Programs	64.4
	100.0

4. By Laboratory:

	Total Program (%)
Ames Laboratory	9.7
Argonne National Laboratory	22.0
Brookhaven National Laboratory	11.0
Idaho National Engineering Laboratory	0.5
Illinois, University of (Materials Research Laboratory)	3.2
Lawrence Berkeley Laboratory	7.2
Lawrence Livermore Laboratory	1.6
Los Alamos Scientific Laboratory	2.8
Mound Laboratory	0.3
Oak Ridge National Laboratory	21.3
Pacific Northwest Laboratory	2.4
Sandia Laboratory	2.1
Solar Energy Research Institute	0.3
Contract Research	15.6
	100.0

5. By Selected Areas of Research:

	Number of Projects (Total=377) (%)	Total Program $ (%)
(a) Materials		
Polymers	3.2	1.0
Ceramics	20.1	12.0
Semiconductors	9.2	5.9
Hydrides	2.9	2.0
Ferrous Metals	12.5	7.3
(b) Technique		
Neutron Scattering	4.5	12.7
Theory	12.2	8.2
(c) Phenomena		
Catalysis	4.2	3.7
Corrosion	10.0	7.7
Diffusion	7.4	4.2
Superconductivity	5.6	5.7
Strength	17.0	9.4
(d) Environment		
Radiation	8.0	10.8

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	172
13	177
40	179
41	192
62	195
68	199
70	206
74	211
78	220
151	
152	

Ceramics

Carbides

52	187	40	
56	192	47	
67	199	58	
68	202	68	
70	205	89	
93	206	126	
96	208	202	
101	217	205	
111	220	206	
126	332	217	
127	347	220	
131	365	310	
138	379	319	
151	390	320	
152	416	375	
177	420	400	
180	439	406	

Glass

Nitrides

101			
111			
127			
131			
151			
177			
191			
202			
205			
206			
208			
316			
338			
347			
352			
365			
379			
416			
420			
437			
439			

Oxides

6	110	201	377
11	111	202	379
35	114	205	383
36	126	206	388
39	131	213	389
47	133	215	395
52	134	220	398
56	135	221	399
57	137	223	404
58	138	233	407
61	139	301	411
67	151	315	418
68	152	316	419
70	177	318	431
87	180	323	432
88	187	327	435
93	194	355	437
96	195	363	
98	197	365	
101	198	367	
109	199	368	

Composites

24	202	341
81	206	347
136	209	351
177	211	354
192	337	392
195	340	436

Fast Ion Conductors

47	122	209
56	135	305
57	192	309
64	195	327
68	198	368
89	199	373
113	201	378
115	202	388
	207	437

Graphite, Carbon, and Coal

2	61	148	206
3	90	151	207
7	101	156	351
13	126	178	352
32	136	192	353
35	139	202	396
39			

Hydrides

7	56	88	119	206
21	62	94	120	305
23	67	98	151	348
25	69	102	190	382
26	70	104	192	
41	74	115	199	
45				

Intermetallic Compounds

24	56	81	151	196
25	57	86	185	202
33	60	126	190	205
42	67	129	191	206
46	69	132	192	209
48	70	146	193	312
50	71	148	195	

Ionic Crystals

56	139	194	205
57	145	195	220
63	190	198	380
86	191	199	419
87	192	202	437
96			

Liquids & Amorphous Materials

22	73	140	172	207	324
36	75	141	174	209	326
37	80	142	185	212	346
56	89	148	196	215	352
61	95	151	199	218	385
63	97	153	202	302	422
66	126	166	205	308	426
71	134				

Metals

Alkali

18	145
71	149
73	151
90	202
92	205
126	328
127	431
142	

BCC Refractory

1	33	122	176	205	408
2	34	125	181	219	412
3	36	126	184	317	442
4	45	127	192	322	
7	48	128	193	335	
12	71	140	195	345	
13	101	145	197	350	
14	104	146	200	386	
19	109	151	201	393	
21	120	154	202	405	

Ferrous

2	79	180	200	317	370	421
3	126	181	201	324	371	424
7	127	182	202	325	374	425
8	129	183	203	329	376	434
9	137	186	205	335	386	
12	146	188	210	339	390	
15	151	190	216	342	394	
35	153	191	218	362	397	
54	154	192	225	364	409	
71	155	195	304	366	413	
73	167	197	314	369	415	
76						

MHD Materials

6	110	195
68	131	318
70	151	355
93	194	363

Polymers

102	176	344
103	186	351
115	194	410
117	202	413
126	306	414
150	337	430
169	341	

Rare Earth Metals and Compounds

1	28	68	165	206
3	33	69	190	220
7	41	70	191	307
14	46	78	192	348
15	56	86	195	
17	57	111	199	
21	62	146	202	
27	67	148	205	

Semiconductors

1	145	205	349
57	146	213	356
63	152	214	357
80	153	215	387
126	190	226	389
130	192	228	417
132	195	231	423
139	186	233	433
140	199	302	436
141	201	303	438
142	202	323	439
144	204	334	

Acoustic Emission

59
131
135
415

Auger Electron Spectroscopy

1	54	132	199	229	379
8	69	137	202	233	394
9	98	150	204	339	411
22	127	154	215	355	428
39	129	155	216	357	435
42	130	182	217	364	439
50	131	186	218	371	

Computer Simulation

20	95	172	209
37	96	196	320
44	129	198	365
45	145	199	401
63	149	202	424
64	151	204	429
68	154		

Elastic Constants

6	120
12	129
13	131
14	378
45	412

Electron Microscopy

7	60	129	181	202	310	342	390
14	69	130	182	205	312	348	391
19	79	131	186	206	314	355	393
44	80	132	187	209	317	362	398
45	81	135	188	213	318	365	409
47	85	137	194	215	322	367	416
48	101	138	195	217	331	374	421
49	107	139	196	219	332	376	428
50	126	150	197	223	334	377	426
51	127	154	198	226	339	386	442
54	128	178	201	301			

Electronic Structure

92
98
119

Electron Spin Resonance

58	195	407
61	186	432
63	198	
113	226	
142	309	
194	383	

Field Emission and Ion Microscopy

39	352
45	377
49	397
333	405

High Temperature Heat Capacity

36
184
429

Infrared Spectroscopy

63	150	214	383
91	194	226	384
140	196	343	388
142	198	373	

Internal Friction

7	133
44	327
104	338
120	345
131	412

Ion Channeling, Scattering and Implantation

19	94	202
49	130	203
50	193	204
51	196	205
54	199	226
69	201	317

Laser Beam Scattering

61	202
117	205
141	222
196	314
199	326
201	378

Low Temperature Specific Heat

1	46	148
15	59	184
20	66	185
24	70	324
26	115	373

Magnetic Susceptibility

Neutron Scattering

Nondestructive Evaluation

(See under Phenomena)

Nuclear Magnetic Resonance

Optical Spectroscopy

7	117	202	384
25	130	205	387
36	141	214	388
58	142	215	392
69	144	223	395
76	194	226	400
91	196	302	433
96	198	383	

Positron Annihilation

45	130
92	205
96	350

Sputtering

48	199	214	221
60	202	215	223
63	205	217	423
69	206	218	

Synchrotron Radiation

25	90	180
61	91	207
62	98	346
63	116	

Theory

4	62	131	175	209	320	356	381	441
5	63	134	186	219	336	358	385	
29	64	142	196	223	337	359	396	
30	75	145	197	303	341	362	401	
31	77	146	198	304	346	366	424	
45	81	151	199	311	349	367	426	
47	116	171	202	314	353	374	438	
49	129	172	205	315	354	375	440	

Thermal Conductivity

Thermodynamics

X-Ray Photoelectron Spectroscopy

X-Ray Scattering

Catalysis

32	61	114	145	204	349	390
33	64	124	146	205	353	403
34	67	126	155	206	358	405
39	69	134	175	229	361	435
42	76	139	199	233	381	440
59	98	140	202	323	389	

Channeling

183	208
202	210
205	226

Corrosion

8	108	154	215	351	393
12	133	183	218	352	400
36	137	202	225	353	402
54	138	205	325	370	406
68	139	208	329	371	407
76	152	210	339	372	409
99					

Crystal Structure, Atomic Distribution and Crystal Transformations

5	62	91	133	180	201	324
6	63	95	134	181	202	367
10	64	98	145	185	204	382
12	67	117	146	190	205	383
14	72	121	147	191	207	384
40	76	126	151	192	215	400
41	81	127	172	195	217	401
46	87	129	176	196	220	423
47	88	130	178	198	310	428
56	90	131	179	199	318	437

Diffusion

Dislocations

Erosion

Electron and Ion Conduction

Electronic Structure

Magnetism

Materials Preparation and Characterization

Nondestructive Evaluation

Phonons

Photovoltaic and Photothermal Phenomena

Point Defects

Precipitation

Recovery and Recrystallization

10	182	220
44	196	382
126	199	424
129	201	
130	202	
131	205	

Sintering

11	133	391
110	135	404
111	151	416
131	206	420
132	365	

Solidification

4	177	205
14	195	206
16	196	315
56	201	378
130	202	

Strength Fracture

2	102	313	362	431
6	105	317	364	434
7	126	324	374	
8	127	335	394	
9	129	337	399	
12	131	338	406	
13	182	341	413	
19	197	345	415	
23	200	351	419	
52	216	354	421	
85	304	359	425	

Constitutive Equations

43	318
44	331
129	336
131	414
306	424

Fatigue

9
52
85
129
131
314
325
364
374
408
421

Creep

44 362
85 365
129 369
131 414
133 418
182 419
186 421
219 425
313 432
322 441
355

Flow Stress

12 322
105 330
127 342
129 345
131 364
133 374
138 386
167 399
194 412
318 425

Stress-Corrosion Cracking

8
25
33
79
152
216
225

Superconductivity

4 62 146 205
14 64 148 217
21 67 175 307
24 86 185 321
29 93 190 324
31 94 191 340
46 97 192 343
56 98 193 354
57 132 199 392
59 143 200 427
60 145 202

Surface Phenomena and Thin Films

1	64	123	183	222	352	402
22	69	130	196	223	356	403
24	72	137	199	224	358	405
25	76	140	201	226	361	407
29	80	141	202	229	367	411
30	91	145	203	233	370	428
37	92	146	204	307	376	433
39	94	149	205	311	377	435
42	95	153	206	317	379	439
54	97	154	214	326	381	440
56	98	155	215	339	393	
60	118	169	218	348	396	
61	119	175	221	349	401	

Welding

100
129
188
325
366
409

Gas

Oxidizing		Hydrogen			Sulphur-Containing
6	194	7	152	348	72
51	202	9	155	361	137
54	205	13	169	364	138
69	208	21	181	381	139
127	215	22	199	389	151
128	216	23	202	390	183
130	218	26	205	394	202
133	339	45	206	397	205
137	355	51	214	408	217
138	370	62	215	434	218
139	393	63	226		370
151	407	98	234		389
155	418	104	304		393
181	428	139	323		409
183	432	151	335		

Magnetic Field

14	67
15	81
27	148
40	190
41	191
46	192
56	307
60	356
62	427

Pressure
Above Atmospheric

28	155
56	170
59	172
103	190
117	191
122	355
147	384
148	

Radiation

Electron		Ion			Neutron		Photons	Theory	Gamma
47	139	19	199	442	19	219	25	95	58
48	186	47	201		21	310	67	102	323
49	199	48	202		48	322	96	186	382
50	202	49	203		56	333	130	199	395
51	205	50	205		67	383	140	202	406
58	233	51	219		186		200	205	
69	310	58	220		196		201	441	
96	312	69	222		199		202		
97	316	130	226		200		205		
120	386	166	310		201		214		
125	391	171	312		202		223		
126	395	186	333		203		382		
130	442	196	391		205				

Temperature

Very Low Temperatures

1	143	202
15	145	203
59	148	205
60	184	308
62	185	330
66	190	340
70	191	343
81	192	347
129	193	358
132	199	373
142	200	

High Temperatures

1	38	138	194	379
2	62	139	195	380
3	68	146	199	399
4	71	151	202	416
6	78	152	205	429
7	85	155	206	
8	98	165	208	
9	103	172	209	
11	128	177	315	
12	131	182	318	
13-	133	184	328	
16	134	190	332	
17	135	191	338	
36	137	192	369	

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