DOE/ER-0013

Materials Sciences Programs

FISCAL YEAR 1978

OFFICE OF BASIC ENERGY SCIENCES

U.S. Department of Energy
Office of Energy Research

September 1978

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FISCAL YEAR 1978

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U.S. Department of Energy
Office of Energy Research
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FOREWORD

On October 1, 1977 a new Department of Energy was established. The Energy Research and Development Administration was transferred to the Department of Energy together with other agencies and parts of agencies within the Federal government. The organizational structure of the new Department of Energy is given in an accompanying chart. The Offices of Basic Energy Science and High Energy and Nuclear Physics report 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, Nuclear Sciences, Engineering, Mathematical and Geosciences and Exploratory Energy Concepts 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 1978 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 1978 funding level, title, personnel, budget activity number (e.g., 01-2), and key words and phrases accompany the project number. The first two digits of the budget number refer to either Metallurgy and Ceramics (01), Solid State Physics (02), or Materials Chemistry (03). The budget numbers carry the following titles:

01-1 - Structure of Materials
01-2 - Mechanical Properties
01-3 - Physical Properties
01-4 - Radiation Effects
01-5 - Engineering Materials

02-1 - Neutron Scattering
02-2 - Experimental Research
02-3 - Theoretical Research
02-4 - Particle-Solid Interactions
02-5 - Engineering Physics

03-1 - Chemical Structure
03-2 - Engineering Chemistry
03-3 - High Temperature and Surface Chemistry

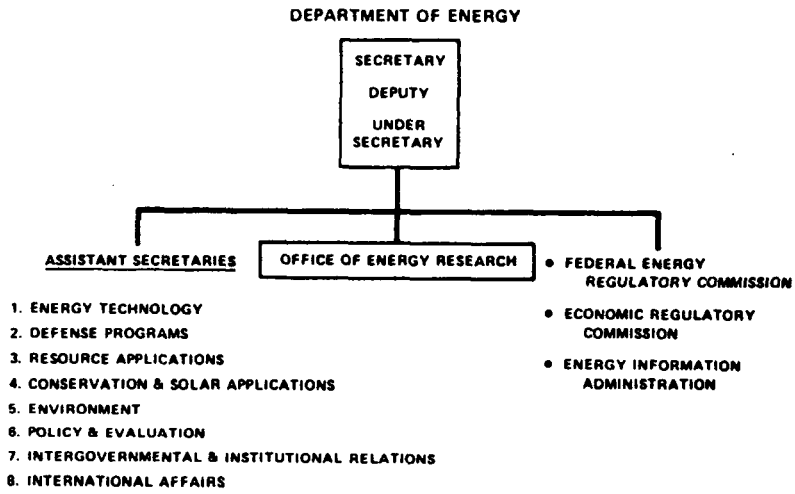
Section C summarizes the total funding level in a number of selected categories. Obviously most projects can be classified under more than one category and, therefore, it should be remembered that the categories are not mutually exclusive.

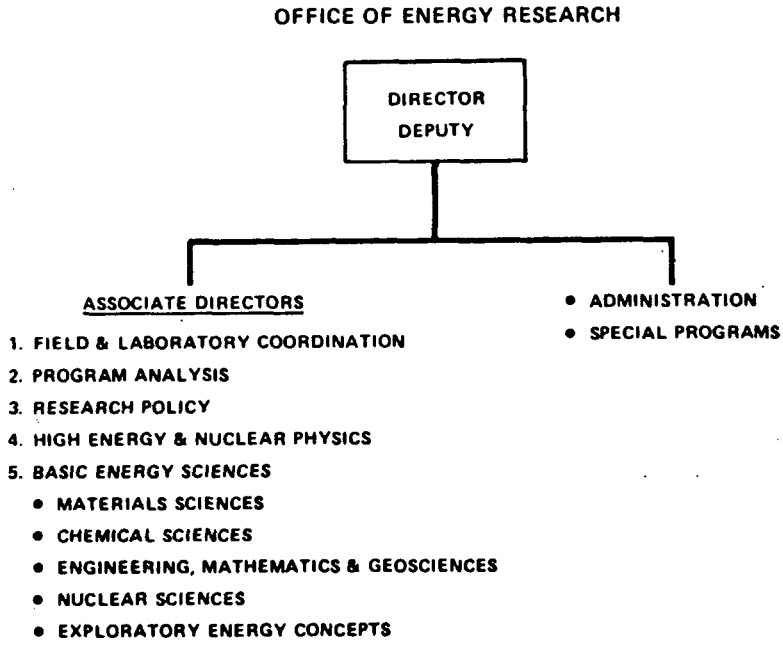
In Section D the references are to the project numbers appearing in Sections A and B and are grouped by (1) investigators, (2) materials, (3) technique, (4) phenomena, and (5) environment.

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

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

ORGANIZATION OF THE DEPARTMENT OF ENERGY



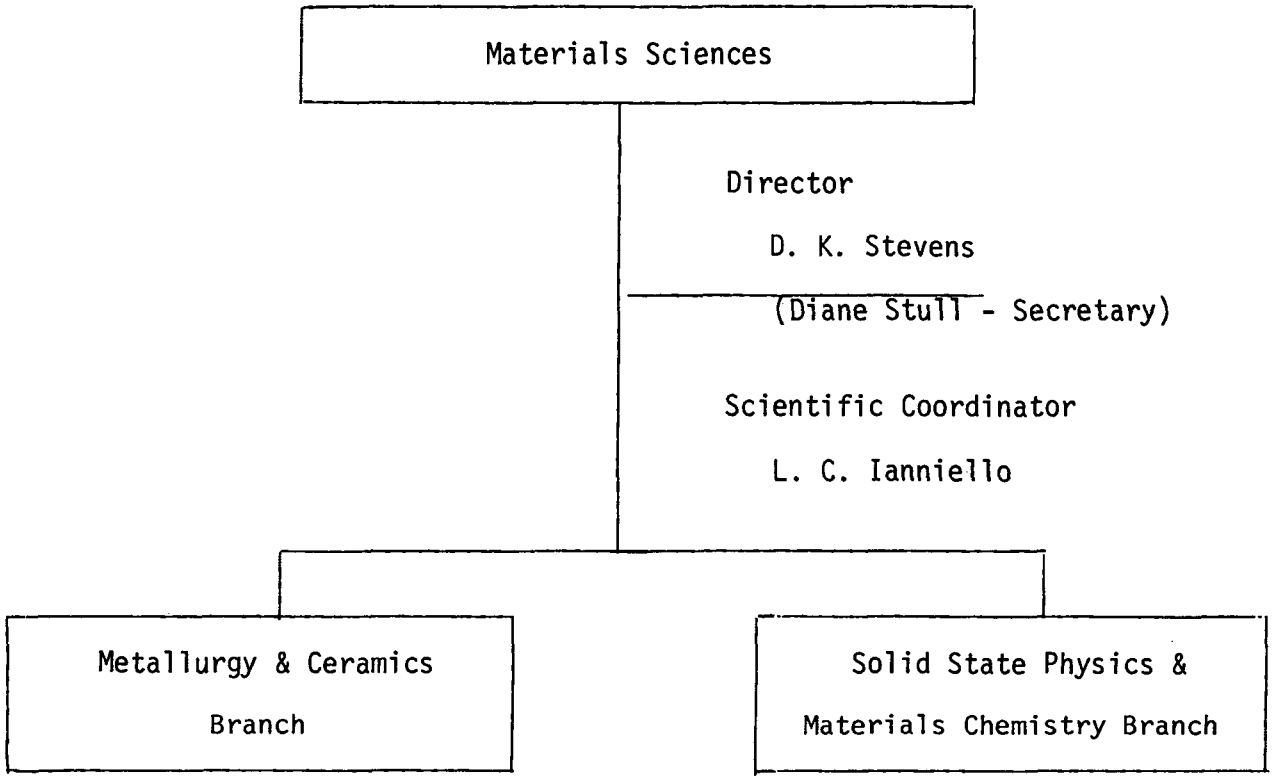


STRUCTURE

OF THE

DIVISION OF MATERIALS SCIENCES

Office of Basic Energy Sciences



Notes: 1/ Returned to Pacific Northwest Laboratory - 9/78
2/ On Leave from Ames Laboratory
3/ On Leave from Georgetown University
4/ On Leave from Los Alamos Scientific 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-
K. A. Gschneidner, Jr. - Phone: (FTS) 865-2272 or 515-294-2272

1. PHOTOVOLTAIC AND THERMOELECTRIC MATERIALS — $113,000 — 01-1
B. J. Beaudry, K. A. Gschneidner, Jr., F. A. Schmidt, R. K. Trivedi, D. E. Williams

Preparation of Schottky barrier-type solar cells by the ultra high vacuum deposition of thin films of semiconducting materials on metal substrates and characterization of the resulting devices; current work involves silicon films on tantalum, tungsten and hafnium substrates. Investigation of the application of rare earth sulfides as high efficiency photovoltaic and thermoelectric materials; heat capacity and optical properties are being studied as a function of changing atomic number in a series of rare earth sesquisulfides. Theoretical and experimental studies of the effects of growth rate and impurities upon the defect structure of photoelectric materials.

2. HIGH TEMPERATURE AND HIGH STRENGTH MATERIALS — $109,000 — 01-1
O. N. Carlson, F. A. Schmidt, R. K. Trivedi

Determination of phase relationships in ferritic alloys and the investigation of microstructural characteristics responsible for their favorable mechanical properties. Studies concerning the migration, due to thermotransport and chemical diffusion, of interstitial solutes in complex, high strength alloys. Surface self diffusion coefficients are being measured for vanadium and other refractory metals at high temperatures. The effects of temperature and interstitial concentration on the strain rate sensitivity and the critical resolved shear stress in vanadium are being studied.

3. PREPARATION AND CHARACTERIZATION OF HIGH PURITY MATERIALS — $218,000 — 01-1
B. J. Beaudry, O. N. Carlson, K. A. Gschneidner, Jr., F. A. Schmidt

Preparation of ultra pure metals and the study of effects of trace impurities on properties. Determination of diffusion and electrotransport behavior of oxygen and nitrogen in thorium and the rare earths. The relationship between atomic size and activation energies for diffusion is being developed for solutes in α and β thorium. High purity rare earth alloys in both single crystal and polycrystalline form are prepared to provide materials for critical scientific programs at Ames Laboratory and other sites.

AMES LABORATORY
Metallurgy and Ceramics -01- (Continued)

4. MECHANICAL PROPERTIES OF CERAMICS $124,000 01-2
O. Hunter

Development of stabilized and partially stabilized oxides with improved mechanical properties for application in MHD systems, batteries, coal gasification reactors and other energy generating schemes; ZrO_2 and HfO_2 are being studied currently. The nature of the electrical conductivity of stabilized ZrO_2 and HfO_2 is being evaluated with the objective of determining ways to decrease the ionic conductivity and increase the electronic conductivity thus minimizing the possibility of electrolytic decomposition of the oxides were they to be placed in service as electrodes for MHD channels.

5. METAL HYDRIDES AND HYDROGEN IN METALS $290,000 01-2
D. T. Peterson, T. E. Scott

Studies are being conducted of the mechanisms involved in hydrogen attack and hydrogen embrittlement in an effort to develop methods for alleviating the often catastrophic effects which hydrogen and its isotopes have on some metals; work is specifically concerned with the refractory metals and steels. Vanadium, niobium and tantalum doped with nitrogen or oxygen are being tested to determine the effects of interstitial atoms on the hydrogen embrittlement of refractory metals. Bonding studies of metal hydrides, using photoelectron spectroscopy, and the consequent determination of the electron energy levels associated with hydrogen in metals are being conducted. Thermotransport measurements for hydrogen and duterium in vanadium and other refractory metals are being made to yield information regarding the heat of transport (Q^*) and the effective charge (Z^*) in these systems.

6. STRESS CORROSION STUDIES $26,000 01-2
T. E. Scott

Microstrain experiments are being initiated as part of an interdisciplinary effort to understand stress corrosion cracking; planned work includes localized plastic deformation studies, and the observation of surface as well as near-surface characteristics of alpha brass under stress in air and ammoniacal solutions.

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

Initial experiments are being conducted concerning the use of shape-memory alloys for low temperature heat engines. Thermomechanical treatments have been developed which permit the fabrication of tube shapes of Ni-Ti shape-memory alloy. Transformation studies and the determination of the effects of mechanical treatment and composition changes on the shape-memory characteristics and fatigue life are planned.

8. DIFFUSION AND FABRICATION STUDIES OF CERAMIC SYSTEMS — $60,000 — 01-3
M. F. Berard

Development of methods for producing sintered refractory oxides (pure and doped) of near theoretical density; current work involves Gd_2O_3, Er_2O_3, Y_2O_3, Sc_2O_3, Eu_2O_3 and Eu_2O_3 doped with HfO_2 and MgO. Investigations concerning the diffusion of Hf and Er in pure and HfO_2-doped Er_2O_3, self-diffusion of Gd in Gd_2O_3, and thermally induced diffusion in CaF_2-SrF_2 and CaF_2-YF_3 systems. Study of interface reactions between tantalum and Er_2O_3.

9. ALLOYING AND PHASE CONTROL STUDIES — $135,000 — 01-3
O. D. McMasters, K. A. Gschneidner, Jr.

Studies of the influence of electron concentration and magnetic impurities on the density of states curve for scandium; electronic specific heat constants are determined for zirconium, magnesium and iron additions. Low temperature heat capacity measurements of $(La_{3-x}R_x)$ $(In_{1-y}M_y)$ materials at zero and high magnetic fields are conducted to determine the effects of alloying and magnetic field on the superconducting transition temperature.

10. CONTROL OF MICROSTRUCTURE AND SOLIDIFICATION STUDIES — $181,000 — 01-3
J. D. Verhoeven

Development of methods for the production of superconducting wire by the application of solidification techniques and phase transformation control; Nb_3Sn and Nb_3Sn-Cu composites are being studied. Directional solidification studies of Pd-Cd, Nb-Ti-Th, and Nb-Ti-Y alloys are planned in an effort to produce useful superconducting wires from these systems.

11. INTERSTITIAL SOLUTE EFFECTS — $70,000 — 01-3
K. A. Gschneidner, Jr., J. F. Smith

Effects of hydrogen on the elastic behavior of Group V metals. Study of the effects of oxygen on the elastic behavior of vanadium over the temperature range 4.2-300 K. Effects of hydrogen on the electronic specific heat constant and Debye temperature of Lu metal are being studied and the influence of hydrogen, nitrogen, oxygen, and carbon on the low temperature heat capacity of Lu will be observed.

12. DETERMINATION OF PHASE DIAGRAMS BY USE OF COMPUTERS — $56,000 — 01-3
D. M. Bailey, J. F. Smith

Calculation of multicomponent phase equilibria from binary thermodynamic data. Perfection of computer programs to generate phase diagrams for binary, ternary and quaternary systems and extension of methods to quinary and higher order systems.

AMES LABORATORY
Metallurgy and Ceramics -01- (Continued)

13. PREPARATION AND PROPERTIES OF RARE EARTH COMPOUNDS AND SINGLE CRYSTALS — $98,000 — 01-3
K. A. Gschneidner, Jr., O. D. McMasters

Preparation of rare earth single crystals and intermetallic compounds by horizontal levitation zone melting, the Bridgman technique, and the strain-anneal recrystallization method. Resulting Crystals and compounds are used as specimen materials in numerous other physical and mechanical property investigations both within the Ames Laboratory and off site.

14. THERMODYNAMIC STUDIES — $18,000 — 01-3
P. Chiotti

Basic thermodynamic measurements in the uranium-mercury system are being conducted to resolve discrepancies contained in the literature and because of possible interest in this system for fuel reprocessing applications. An effort has been maintained to develop a process for the removal of pyrite sulfur from coal based on the high pressure oxidation of the pyrite.

15. MAGNETIC MATERIALS — $42,000 — 01-3
C. W. Chen

Amorphous iron alloys are being evaluated in a search for materials with saturation magnetization values greater than 16,000 gauss; glassy films or ribbon of $Fe_{1-x}G_x$ systems (where G is the glass-forming constituent) are being prepared and will be subjected to coerceive force, remanence, permeability and energy loss studies.

16. DOPED ALUMINUM THIN FILM SOLAR COLLECTORS — $42,000 — 01-3
C. W. Chen

Spectrophotometric studies on thin films of aluminum doped with Si, Mn, Zn, Ge or Ag; determination of the efficiency of these materials as solar energy collectors.

17. ORDERED ALLOYS — $98,000 — 01-3
F. X. Kayser

Studies of the mechanical properties and elastic constants of Ni_3Al:Ni_3Ti are being conducted with the objective of understanding the strengthening mechanisms which are operating in nickel base superalloys. Lattice parameter vs. composition studies of ferromagnetic DO_3-ordered Fe-Al-Si alloys; these materials are expected to have superior soft magnetic properties.

AMES LABORATORY
Metallurgy and Ceramics -01- (Continued)

18. HELIUM BUBBLE, VOID, AND DEFECT DEFECT CLUSTER FORMATION — $118,000 — 01-4
C. W. Chen

Development of methods for suppressing void formation in neutron-irradiated metals by vacancy trapping with carbon atoms. Effects of Zr and Be solute atoms on the formation of He bubbles in Ni++ - irradiated V-Ti alloys; the morphology and distribution mode of the He gas bubbles are being studied as functions of alloy composition and damage profile. Study of geometry and dislocation characteristics of interstitial clusters in neutron-irradiated Nb.

19. RADIATION HARDENING THEORY — $46,000 — 01-4
M. S. Wechsler

Computer simulation studies analyzing the dependence of radiation-induced increase in yield stress on the density and size distribution of defect clusters.

20. RADIATION DAMAGE IN METALS AND ALLOYS — $36,000 — 01-4
M. S. Wechsler

Electron irradiation of vanadium; the oxygen trapping by defect clusters produced by 3 MeV electrons is being evaluated and compared to the effects observed earlier in the neutron-irradiated material. Tensile tests are being conducted on neutron-irradiated thorium and thorium carbon alloys as part of the study of the effects of irradiation on the mechanical properties of thorium.

21. NON-DESTRUCTIVE EVALUATION — $70,000 — 01-5
C. P. Burger, K. G. McConnell,
L. W. Schmerr, J. F. Smith, D. R. Wilder,
L. W. Zachary

Project was initiated during FY 1978. Work involves flaw characterization by ultrasonic spectroscopy and the boundary integral equation method to provide a basis for evaluating internal flaws in materials in service situations. Method will be developed that use ultrasonic Rayleigh waves for the quantitative evaluation of surface cracks and breaking near surface flaws. A method for the non-destructive evaluation of the tension in large bolts has been perfected; the technique is based on the measurement of ultrasonic wave velocities by the pulse-echo-overlap method.

AMES LABORATORY
Solid State Physics Division -02-
K. L. Kliewer - Phone: (FTS) 865-4037 or 515-294-4037

22. NEUTRON SCATTERING $340,000 02-1
W. A. Kamitakahara, J. Khatamian, G. R. Kline, C. Stassis

Study of the thermodynamic properties and structural transformations of solids at high temperatures (Zr, Ti, Tc); effect of hydrogen and carbon impurities in metals (Th-C, Th-H, Y-H); electron-phonon interaction and its relation to superconductivity (La_3S_4, La); mixed valence compounds ($CeSn_3$, γ-Ce).

23. MAGNETIC PROPERTIES OF SOLIDS $54,000 02-2
S. Legvold

Experimental magnetic studies of localized and conduction band electrons in rare earth alloys; Seebeck effect near the Lifshitz bicritical point of alloys (Gd-Y, Gd-Sc, Tb-Th); magnetic ordering temperatures of light rare earth alloys (Ce-La, Nd-La); crystal field effects in light-heavy rare earth single crystals (Tb-Pr, Dy-Pr); spin disorder scattering in cubic La alloys (La-Gd, La-Tb, La-Dy, etc.); easy direction of magnetization for Er.

24. NUCLEAR RESONANCE IN SOLIDS $176,000 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, $CsScCl_3$, $BaVS_3$).

25. SUPERCONDUCTIVITY $320,700 02-2
D. K. Finnemore, T. Y. Hsiang, J. W. Osmun, J. E. Ostenson, E. L. Wolf, R. J. Noer

Superconductivity in A-15 composites having dimensions on the order of 100 Å. Electron tunneling of strong-coupling transition metal, transition-metal alloy, and transition-metal compound superconductors using ultra-thin normal-superconductor proximity junctions; preparation and investigation of oriented (Pb-Cd and Nb-Th), superconductor-normal metal, composites by directional solidification; critical currents and critical magnetic fields in Nb-Th and Nb-Y superconductor-normal metal composites; flux pinning and thermal transport. Auger analysis and photoemission of getter sputtered and surface grown V_3Ga and other A-15 superconducting films.

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

26. THERMODYNAMIC AND TRANSPORT PROPERTIES OF SOLIDS — $410,400 — 02-2
M. S. Anderson, A. J. Bevolo
G. C. Danielson, H. R. Shanks,
C. A. Swenson

Electrocatalytic activity of tungsten bronzes (Na_xWO_3); capacitance-dilatometer thermal-expansion measurements on amorphous solids at low temperatures (organic polymers, fused silica); high pressure studies of the heat capacities of solid hydrogen and solid deuterium, and of the equations of state of the alkaline earth metals; growth of crystals of tungsten bronzes (Na_xWO_3, K_xWO_3, H_xWO_3, Rb_xWO_3) and layer compounds ($NbSe_2$, $TaSe_2$, NbS_2, InSe, InTe); electrical resistivity, thermal conductivity and Seebeck coefficient of high purity vanadium and tantalum; low temperature heat capacity of perovskite compounds.
SURFACE ANALYSIS LABORATORY: Auger and SIMS studies of surfaces and interfaces: surface composition and depth profiles of tungsten bronzes (Na_xWO_3, H_xWO_3, Pt-doped Na_xWO_3); corrosion of surfaces; evaporated and sputtered thin films, Schottky-barrier, and metal-oxide-semiconductor interfaces; Schottky-barrier solar cells; amorphous silicon-metal interfaces; ohmic contacts.

27. OPTICAL AND SPECTROSCOPIC PROPERTIES OF SOLIDS AND LIQUIDS — $188,900 — 02-2
T. E. Furtak, A. Habenschuss,
D. W. Lynch, C. G. Olson,
F. H. Spedding, R. Rosei,
J. H. Weaver

Optical properties (transmission, reflection, 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, noble metals, II, and II-VI semiconductors. Photoemission into liquid electrolytes, electrochemical modulation spectroscopy, microspectro-electrochemistry, and photoelectrochemistry: binary alloys susceptible to localized corrosion, surface excitation, and adsorption phenomena on model systems (e.g., noble metals). Photoelectrolysis. Infrared and visible emissivity at high temperatures of materials suitable for photothermal conversion and other solar energy applications; transition-metal alloys, Al-Fe alloys, superalloys. Optical properties of rare earth chelates for solar cell applications. Raman scattering and x-ray diffraction in aqueous solutions. HDO, D_2O and rare earth chlorides and perchlorates. Raman scattering from adsorbates (hetercyclic amines on noble and transition metals).

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

28. OPTICAL AND SURFACE PHYSICS THEORY — $157,500 — 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; collective excitations: phonons, plasmons, and excitons. Photoemission with emphasis on effects associated with the presence of a surface, evanescent and 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 absorbers, and optical properties of phase-change materials for solar applications.

29. SUPERCONDUCTIVITY THEORY — $66,800 — 02-3
E. H. Brandt, J. R. Clem, R. A. Klemm, K. Machida

Properties of magnetic flux in type-I and type-II superconductors; induced voltages and energy dissipation due to flux motion, flux vortex nucleation, and surface pinning; behavior of arrays of non-parallel vortices; critical currents and flux pinning in inhomogeneous superconductors; instabilities; ac losses; 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; static and dynamic properties of spin glasses.

30. MAGNETIC AND ELECTRONIC PROPERTIES OF SOLIDS THEORY — $135,700 — 02-3
B. N. Harmon, S. H. Liu

Electronic properties of transition metals and compounds (ScH_2, YH_2, ZrCl, $NaWO_3$, $PtWO_3$). Theory of soft modes, phonon anomalies, charge density waves, and displacive lattice transformations and their relation to the electron-phonon interaction and superconductivity (e.g., Nb, NbC, Zr, Na_xWO_3). High temperature materials and properties including bonding, melting, and ion transport. Thermal fluctuation and energy transport in thin films (1/f noise). Induced and intrinsic magnetization densities in metals (Gd, Cr, Pd, Lu), compounds, and alloys, spin waves and other excitations in disordered magnetic systems: the d-f exchange interaction in rare earth-metallic materials. Modeling of the metal-electrolyte interface.

AMES LABORATORY
Materials Chemistry Division -03-
J. D. Corbett - Phone: (FTS) 865-3086 or 515-294-3086

31. X-RAY AND NEUTRON CRYSTALLOGRAPHY $214,000 03-1
R. A. Jacobson, J. E. Benson,
B. J. Helland

Development of diffraction techniques and service facilities especially those designed for the novice user; 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; diffraction studies of coal-quantitative identification of mineral species on-line; radial distribution function analysis of coal's amorphous scattering.

32. METAL-METAL BONDING IN SOLID STATE MATERIALS $129,000 03-1
J. D. Corbett

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 of new types of reduced compounds; stress-corrosion-cracking by zirconium iodides; homopolyatomic ions (e.g., of Ge, Sn, Sb, Bi, Te); ionic intermetallic phases.

33. CHEMISTRY OF HEAVY TRANSITION METALS $147,000 03-1
R. E. McCarley, V. Katovic

Chemistry of heavy transition elements, especially Nb, Ta, Mo, W, controlled synthesis and characterization of compounds with strong metal-metal bonds in dimers, clusters, and extended structures; electronic structure related to properties and reactions of metal clusters; catalytic applications; compounds with unusual reactivity.

34. METALS FROM FLY ASH $115,000 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.

35. LIQUID METALS $57,000 03-2
R. G. Bautista

Heat capacities and heat content of liquid Cu-Ce alloys. Correlation and prediction of liquid alloy heat contents.

AMES LABORATORY
Materials Chemistry Division -03- (Continued)

36. EMITTANCE PROPERTIES OF MATERIALS AT HIGH TEMPERATURES — $41,000 — 03-2
R. G. Bautista

Normal spectral emittance of liquid iron, nickel, and Cu-Ce alloys. Practical temperature measurements by optical pyrometry.

37. CORROSION AT HIGH TEMPERATURES — 03-2
R. G. Bautista

Modelling of corrosion of high chromium alloys by O_2 and SO_2 including scale resistance and chemical reactions. To be initiated in FY 1979.

38. PARTICULATE PROCESSING — $107,000 — 03-2
L. E. Burkhart

Particle and fluid motion in mass transfer systems by high-speed photography; experimental techniques, and mathematical modeling; transport near interfaces, especially drops, bubbles, and solid particles; theoretical analysis, kinetics and control of particle size distribution, growth rate, and morphology in operations involving the preparation of ceramic powders; reaction kinetics and mixing in multicomponent mass transfer systems involving chemical reactions with emphasis on correlation between theory and experiment.

39. HIGH TEMPERATURE CHEMISTRY — $167,000 — 03-3
H. F. Franzen, A. V. Hariharan
J. Anderegg, C. E. Myers

Structure and bonding in refractory and corrosion-resistant compounds, particularly metal-rich transition metal chalcogenides, phosphides and aluminides; high temperature stability, phase equilibria and electronic properties; X-ray photoelectron spectroscopy and band structures of refractory solids; X-ray diffraction and mass spectrometry at high temperatures.

40. SURFACE CHEMISTRY AND CATALYSIS — $293,000 — 03-3
R. S. Hansen, B. C. Gerstein,
K. G. Baikerikar, T. Taki

Heterogeneous catalysis by metals and metal oxides. Reactions at clean surfaces associated with coal liquifaction and gasification. Field emission, flash desorption, LEED and Auger spectroscopy. Single crystal face catalysis. Electrical double layer properties and their alteration by adsorption. Mechanical flow properties of interfaces. Pulse and multiple pulse NMR studies of surface sites and of electronic structures of adsorbed molecules on high surface area substrates. Heteronuclear dipolar oscillation NMR and geometries of absorbed molecules.

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

Materials Science Division -01-
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F. Y. Fradin - Phone (FTS) 972-4966 or 312-972-4966

41. ALLOY PROPERTIES $284,000 01-1
D. J. Lam, G. S. Knapp, B. W. Veal, Jr., P. Jena, H. Chen

Fundamental studies of electronic structure and its relationship to physical properties and bondings in alloys and compounds. XPS and extended x-ray absorption fine structure studies of the structural and electronic properties of Fe_2O_3 in sodium disilicate glass. XPS study of bonding of uranium in sodium-silicate glasses and the study of electronic structure and hydrogen bonding in transition metal hydrides. Theoretical study of conduction electron polarization in PuP. Theoretical investigation of the systematics in the Knight shifts at nonmagnetic sites in rare-earth-, transition- and actinide-Group V A elements.

42. SCATTERING STUDIES $673,000 01-1
M. H. Mueller, G. H. Lander

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 perovskites and complex hydrides, inelastic neutron experiments on UO_2.

43. ACTINIDE MATERIALS $252,000 01-1
M. B. Brodsky, A. J. Arko

Electronic structure of actinide metals, alloys and compounds; low temperature specific heat; electrical resistivity; and magnetic susceptibility of metallic actinides to study spin fluctuations and band magnetism; de Hass van Alphen effect in actinide intermetallic compounds to determine electronic structure.

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

44. PROPERTIES OF HIGH-TEMPERATURE MHD MATERIALS — $198,000 — 01-1
D. J. Lam, A. T. Aldred,
B. W. Veal, Jr., D. P. Karim

Experimental and theoretical studies of the lattice and electronic structure of ceramic materials for very high temperature applications; electrical conductivity, Seebeck coefficient, and magnetic susceptibility studies of strontium-doped lanthanium chromite; systematic XPS studies of $LaXO_3$-type compounds (X = 3d transition element); theoretical study of the final-state multiplet structure of 3d electronic configurations in cubic crystal environment; relativistic molecular cluster model calculation of XPS spectra of $LaXO_3$-type compounds.

45. CATALYSIS AND SURFACE STUDIES — $191,000 — 01-1
M. B. Brodsky, S. D. Bader,
T. W. Orent

Use of intermetallic compounds as catalysts; electronic and atomic structure of intermetallic compound and transition metal surfaces; effects of gases on surface properties, low energy electron diffraction; x-ray photoelectron spectroscopy; electron loss spectroscopy; and Auger electron spectroscopy.

46. CORROSION STUDIES — 01-1
M. B. Brodsky, R. S. Averback,
O. K. Chopra, T. F. Kassner,
K. Natesan, P. R. Okamoto,
R. L. Lyles, Jr., L. E. Rehn

In-situ studies of alloy corrosion in the High Voltage Electron Microscope; studies of corrosion by low energy electron diffraction, Auger electron spectroscopy, x-ray photoelectron spectroscopy, electron loss spectroscopy, kinetic studies and ion-beam analysis; alloy modification by ion beam implantation for corrosion studies; effects of stress on oxidation and sulfidation. To start in FY 1979.

47. CONSTITUTIVE RELATIONS — $264,000 — 01-2
U. F. Kocks, J. L. Routbort,
A. P. L. Turner, T. Hasegawa

Theoretical and experimental search for unifying constitutive relations describing the kinetics of flow and strain hardening, recovery and stress relaxation, creep and fatigue, over a wide range of strain rates, especially at high temperatures. Characterization of the dislocation structure of deformed specimens by TEM and x-ray scattering techniques. Materials currently investigated: stainless steels, nickel alloys, aluminum, copper, MgO. Application of results to theory of plastic instabilities.

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

48. STRENGTH OF ALLOYS $280,000 01-2
U. F. Kocks, R. A. Mulford,
R. O. Scattergood, R. B. Schwarz

Theoretical and experimental investigation of strengthening mechanisms, especially solution hardening at high temperatures, using mechanical tests, internal friction techniques, and computer simulation. Dislocation theory, including dynamics and statistics. Materials currently investigated: various nickel, aluminum, and copper base alloys.

49. METAL PHYSICS $880,000 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, J. F. Miller
R. P. Gupta

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 positron annihilation spectroscopy, tracer diffusion, resistometry, transmission-electron- and field-ion-microscopy, neutron and X-ray diffraction, and ultrasonic-wave propagation.

50. SUPERCONDUCTIVITY $243,000 01-3
F. Y. Fradin, G. S. Knapp,
P. Jena, H. Chen

Theoretical and experimental research on the electron-phonon interaction with changes in the electron and phonon spectra in various classes of high T_c intermetallic compounds; NMR and Mossbauer effect studies of the interaction of magnetic ions and the superconducting electrons in ternary rhodium-borides and ternary molybdenum-chalcogenides; EXAFS investigation of anharmonic behavior and the effects of defects on the superconducting properties of the A-15 compound V_3Ga; heat capacity and magnetic susceptibility studies of the electron-phonon coupling in C-15 compounds. Theoretical investigation of isotope effect in PdH(D) superconductors.

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

51. BASIC CERAMIC STUDIES $399,000 01-3
N. L. Peterson, W. K. Chen
J. Faber, Jr., M. D. Rechtin,
D. Wolf, and K. K. Kim

Diffusion mechanisms and point defect studies in metal oxides as a function of oxygen pressure at high temperature using tracer diffusion, NMR, Mossbauer, and differential dilatometry techniques; ionic transport mechanisms in sodium beta-alumina; defect-solute interactions in oxides; grain-boundary diffusion in oxides; theoretical studies of kinetic processes in metal oxides and solid electrolytes; neutron and x-ray scattering studies of order-disorder transition in superionic conductors and defect clustering in metal oxides, amorphous alloys and glasses including effects of helium using electron microscopy; oxidation processes in nonstoichiometric oxides using the environmental cell in the HVEM.

52. SOLAR MATERIALS 01-3
D. J. Lam, P. P. Pronko,
M. D. Rechtin, B. W. Veal, Jr.

Fundamental studies of structural and electronic properties of semiconducting materials for possible photovoltaic applications: transmission electron microscopy and nuclear backscattering study of kinetics of regrowth of ion-implanted silicon; ultra-violet and x-ray photoemission spectroscopy study of the electronic band structure of silicon-hydrogen alloys; extended x-ray absorption fine structure study of near neighbor environment of germanium-hydrogen alloys; and the theoretical study of electronic band structure of silicon-hydrogen alloys. To start in FY 1979.

53. NEUTRON IRRADIATION STUDIES $564,000 01-4
T. H. Blewitt, R. C. Birtcher,
B. S. Brown, M. A. Kirk, Jr.
B. A. Loomis, H. Lefakis

Defect cascade production at liquid helium temperature and subsequent annihilation and clustering; flux pinning in superconductors by defect cascades; resistance and critical temperature changes in irradiated A-15 superconductors; characterization of neutron spectrum and damage energy distributions; neutron sputtering, replacement collision sequences; effect of defect saturation on length and resistivity changes; mechanical properties and swelling due to voids in Nb as a function of ion dose, temperature and oxygen content; void nucleation in nickel; radiation enhanced creep; target and irradiation facility design for the Intense Pulsed Neutron Source (IPNS); radiation sources include the CP-5 low temperature facility and the 4 MeV Dynamitron.

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

54. CHARGED-PARTICLE IRRADIATION STUDIES $632,000 01-4
K. L. Merkle, R. S. Averback,
R. Benedek, R. L. Lyles, Jr.
W. B. Jager

Damage function studies by ion irradiation, HVEM, and field ion microscopy; correlations of 14 MeV and fission neutron damage with heavy ion damage in metals; properties of self-interstitial atoms; studies of energy density effects in displacement cascades and sputtering; TEM and HVEM investigations of displacement cascades in binary alloys; interatomic potential calculations; diffusion of implanted hydrogen and helium in metals; defect cluster formation by HVEM. Major experimental facilities: 300keV heavy ion accelerator and High Voltage Electron Microscope with ion interface for future 2 MeV ion accelerator and low energy ion injector.

55. KINETIC STUDIES $729,000 01-4
H. Wiedersich, B. H. Hall
F. V. Nolfi, Jr., P. R. Okamoto,
D. I. Potter, A. Taylor
L. E. Rehn, A. A. Sagues

Investigations into forces and mechanisms that lead to the formation of defect aggregates and precipitates and other inhomogeneous distributions of atoms in solids without and with displacement-producing irradiation; agglomeration of gaseous compounds, e.g., CH_4 which can lead to hydrogen attack in pressure vessels used in coal gasification; solute segregation to voids and free surfaces during irradiation; defect-solute complexes; effects of irradiation on the microstructure of two-phase alloys - dynamic dissolution and reprecipitation; the effect of fine precipitate dispersions, solute additions, and helium on void and dislocation loop formation during ion bombardment; irradiation creep; radiation sources include 300KeV heavy-ion accelerator, 4 MeV Dynamitron -- 2 MeV Van De Graaff Dual-ion-beam Facility, high-voltage electron microscope, and 2 MeV ion accelerator (being procured) for in-situ HVEM studies and ion beam analysis.

56. HIGH VOLTAGE ELECTRON MICROSCOPE-TANDEM FACILITY 01-4
R. L. Lyles, Jr., A. Taylor,
P. P. Pronko

Operations and development of 1.2 MeV High Voltage Electron Microscope Facility with ion beam interface; specimen stages for heating (1000°C), cooling (9°K), straining, specific gaseous environments, in situ ion irradiations with 300 keV ion injector and a 2 MeV Tandem Ion Accelerator which will be operational in 1981; establishment of an external HVEM User Program. Operation to begin in FY 1979.

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

57. NONDESTRUCTIVE EVALUATION $65,000 01-5
M. H. Mueller, E. S. Fisher
K. J. Reimann

Examination of voids, precipitates, and strain fields from impurities in materials by neutron small-angle scattering. Design responsibility for small angle instrument at IPNS. Use of bulk-wave ultrasonics to provide quantitative description of size, shape, and orientation of flaws. Detection of near-surface defects using precise measurements of high frequency ultrasonic surface wave velocities.

58. EROSION AND WEAR $90,000 01-5
A. P. L. Turner, J. L. Routbort
R. O. Scattergood, T. H. Kosel

Experimental investigation of erosion mechanisms by controlled particle impacting and SEM/TEM. Characterization of damage as it accumulates during creep and fatigue. Materials currently investigated: nickel alloys, high-strength steel, MgO, silicon-carbide ceramics.

ARGONNE NATIONAL LABORATORY
Solid State Science Division -02-
D. L. Price - Phone (FTS) 972-5493 or 312-972-5493

59. PULSED NEUTRON SOURCE DEVELOPMENT $350,000 02-1
J. Carpenter, R. K. Crawford,
R. Kleb, R. Kustom,
J. Simpson, N. Swanson

The design and operation of prototypes of the proposed Intense Pulsed Neutron Source (IPNS) and their use for development and testing IPNS instrumentation. The unique pulse source advantages of a large epithermal flux and short pulse width will be exploited for elastic scattering studies of large momentum transfers (up to 80 A) and for inelastic scattering at large energy transfers. Studies also include research and development activity in support of rapid-cycling high-intensity synchrotrons as pulsed-source drivers. Materials and phenomena to be investigated include superconductors, hydrogen-storage materials, candidate MHD electrode materials, solid electrolytes, one-dimensional conductors and amorphous materials, and magnetic processes such as Stoner excitations.

60. NEUTRON SCATTERING STUDIES $1,243,000 02-1
T. Brun, G. Felcher,
R. Kleb, C. Pelizzari,
S. Sinha, J. Jorgensen,
T. Postol, K. Skold,
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 research 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.

ARGONNE NATIONAL LABORATORY
Solid State Science Division -02-

61. MATERIALS PREPARATION AND CHARACTERIZATION — $170,000 — 02-2
S. Susman, D. Hinks

Preparation of research samples of metal, insulator and semiconductor single crystals with documented physical and chemical properties; investigation of mechanisms involved in purification and the development of clean-room facilities and crystal growth techniques, including crystal growth of high-temperature materials and purification with halogen and hydrohalogen gases. Materials of current interest include rare-earth compounds with the CsCl structure for neutron scattering and magnetic studies, refractory oxides such as Y_2O_3 for high-temperature materials research, rare-earth salts such as yttrium ethylsulfate: ytterbium for nuclear polarization experiments, and the alkali halides and cyanides in the orthorhombic phase.

62. DEFECTS IN NONMETALLIC SYSTEMS — $195,000 — 02-2
P. Yuster, C. Delbecq,
S. Marshall

Study of defects and impurities in nonmetallic crystals and the processes caused by exposure of insulators to ionizing radiation. Major areas of activity include: the excitation, tunneling recombination and luminescence processes in heavy-metal impurities in insulators; structure and reorientation dynamics of covalently bonded molecular-ion centers (F_2^-, Cl^-, FCl_2^-, $BrCl^-$) in alkali halides; ESR studies of F_2 centers in alkali fluorides, and manganese in calcite; and production and motion of interstitial molecular-ion species (FCl^-, $BrCl^-$ and ICl^-) in alkali halides.

63. LOW TEMPERATURE STUDIES — $209,000 — 02-2
P. Roach, R. Webb

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 techniques for susceptibility measurements in the low millikelvin range; static and dynamic susceptibility of He^3 phases; and the search for triplet or P-wave superconductivity in metals.

ARGONNE NATIONAL LABORATORY
Solid State Science Division -02-

64. SUPERCONDUCTIVITY STUDIES $308,000 02-2
K. Gray, C. Falco,
H. Willemsen

Research in nonequilibrium processes in superconductors and the relation between metallurgical and superconducting properties in type II materials. Current activities include: studies of quantum interference effects; magnetic structures and transport properties of superconductors using tunnel junctions; superconducting energy gap enhancement by microwaves; thermoelectric transport coefficients in the superconducting state; the preparation of high T_c materials such as Nb_3Sn by high-rate sputtering and studies of flux pinning, critical current density and radiation damage in these new materials; the development of high-temperature SQUIDS and superconducting switches; and studies of superconducting transistor analogues.

65. CATALYSIS AND SURFACE STUDIES $274,000 02-2
D. O'Reilly, G. Crabtree,
L. Iton, G. Felcher,
R. Webb

The dynamics and properties of atoms and molecules adsorbed on surfaces as studied with NMR, ESR and ENDOR spectroscopy; studies of adsorbed species and catalysis in the zeolites, silica gel, the zinc and copper "chromite" systems, and supported metal catalysts; use of benzene and transition metal ions as a probe of active catalytic surfaces; atomic-beam scattering from surfaces; magnetic field effects on surface reactions; and SQUID susceptibility and NMR measurements.

66. ELECTRONIC, MAGNETIC AND LATTICE PROPERTIES $341,000 02-2
G. Crabtree, B. Dunlap,
H. Kierstead, G. Shenoy,
D. Dye, J. Friedt

Studies of the Fermi surface in metals, alloys and intermetallic compounds via the de Haas-van Alphen effect; measurement of conduction-electron effective masses and g-factors; studies of the scattering of electrons by impurities, lattice defects and local moments. Materials of interest include Nb, Pt, and Pd, actinide materials such as U_3As_4, UGe_3, UIr_3 and α-U and rare-earths and superconducting A15 compounds such as Nb_3Sb. Mossbauer effect studies of high-field ternary superconductors such as $SnMo_6S_8$ and related materials; crystal field and spin-relaxation effects in lanthanide and actinide compounds including $Yb_2Ti_2O_7$, $Dy(OH)_3$; defect pinning in Eu-Mg alloys and quadrupole interactions in Hf-Zr alloys. Structural and electronic properties studies of the rare-earth hydrogen-bearing materials ZrH_x, HoH_2, HoD_2, ErH_2, DyH_2 and DyD_2 and rare-earth d-transition metal alloys including Th_7Fe_3 and $Th_7Fe_3H_{30}$. EXAFS studies of small metal molecules isolcated in inert gas matrices.

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

67. LIGHT SCATTERING AND ACOUSTICS — $53,000 — 02-2
P. Roach, C. Falco,
K. Miyano

A program to study low-frequency mechanical and molecular statistical properties of liquids and solids employing light scattering, sound and surface waves. Research areas include ultrasonic propagation and Brillouin scattering studies of shear wave propagation in liquid crystals; wave propagation in monomolecular films on fluids; and development of a tunable Josephson junction source of submillimeter radiation. Materials of interest include P-azoxyanisole and films of alkylalcohols and lecithins.

68. SOLAR MATERIALS — $236,000 — 02-2
L. Guttman, J. McMillan
D. Y. Smith

A multi-disciplinary study of the properties of materials with solar applications. Topics include: study of crystallization and annealing processes in amorphous thin-film semiconductors for optically selective surfaces; properties of heat mirrors; investigation of the random network model of amorphous materials; electronic structure of pure and hydrogenated amorphous silicon; theory of bulk and surface optical properties; and sum-rule constraints on attainable optical properties.

69. ELECTRONIC AND TRANSPORT PROCESSES IN REFRACTORY OXIDES — $211,000 — 02-2
C. Delbecq, D. Hinks,
J. Jackson, S. Marshall,
W. Primak, S. Susman,
P. H. Yuster

Studies of refractory materials including the preparation and characterization of research samples of high-temperature oxides including Y_2O_3; optical and ESR studies of the motion and trapping of electrons and holes and glow-tube studies of ionic transport in conducting oxides and silicates; high-temperature transport measurements. Materials of interest include Y_2O_3, Al_2O_3, yttrium aluminum garnet, A_2O_3:Cr_2O_3 and silicate glasses.

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

70. SOLID STATE THEORY $470,000 02-3
T. Arai, T. Gilbert,
D. Koelling, A. Rahman,
J. Robinson, P. Vashishta,
C. Hsu, K. Lau

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; electronic structure of perovskites; and theoretical studies of superionic conductors including CaF_2 and α-AgI.

71. PARTICLE SOLID INTERACTIONS $260,000 02-4
J. Jackson, W. Primak

Production and recovery of radiation damage by ions, electrons and neutrons in metals and insulators; elementary defects and their interactions; defect production and trapping rates; properties of divacancies and self-interstitial atom clusters and associated strain fields. Metals under study include nickel and the soft superconductor indium. Studies of electromigration at high temperatures in glasses and nonmetal MHD electrodes; studies of surface radiation damage in insulators including work on Al_2O_3, Si_3N_4, SiC, B_4C, ZrO_2, stabilized zirconia, vitreous silica, and glasses; studies of optical and electrical effects and dimensional changes; stress formation and relief migration of implanted ions to surfaces and voids; and blister formation and spallation.

72. ENGINEERING PHYSICS 02-5
C. Falco

Studies of the feasibility of using SQUID magnetometers for geological prospecting for hydrocarbon deposites; high-temperature SQUIDS. To be started in FY 1979.

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

73. NEUTRON SCATTERING, X-RAY AND EXAFS STRUCTURAL STUDIES OF MATERIALS — $640,000 — 03-1
S. W. Peterson, M. Atoji, J. M. Williams, A. H. Reis, Jr., E. G. Sherry, A. J. Schultz, J. Roziere, P. Johnson, R. W. Broach, R. K. Brown, M. Depp, D. Gerrity, J. Kelber, T. Lynch, T. Morrison, K. Stearley

The major goals are to develop new materials with important energy-related properties and to develop property-structure correlations. Utilizing neutron and x-ray diffraction techniques, emphasis is on inorganic and organic compounds with high anisotropic conductivity, on hydrogenation and methanation catalysts, and on magnetic-moment structural studies of rare-earth metals, alloys, and compounds, plutonium and uranium carbides and oxycarbides, and sodium-tungsten bronzes. Extended x-ray absorption fine structure (EXAFS) analysis is being used to investigate graphite intercalates and Fischer-Trophsch catalysts. A single-crystal, pulsed-neutron diffractometer using white-beam Laue techniques and time-of-flight analysis is being developed.

74. CALORIMETRY AND THERMODYNAMICS — $164,000 — 03-3
H. E. Flotow, D. W. Osborne

Heat capacity measurements and determination of entropies, enthalpies and Gibbs energies from 0.1 to 350K for use in thermodynamic calculations at higher temperatures; emphasis is placed on inorganic compounds of importance in energy systems; compounds currently being studies are: PrF_3, NdF_3, $^{242}PuH_2$, $^{242}PuH_3$ and $^{242}Pu_2O_3$. Work on LaF_3, ThH_2 and $ThH_{3.75}$ has recently been completed, and measurements on $LaNi_5H_x$, Cs_3CrO_4 and $LaCrO_3$ are also planned for FY 1979.

ARGONNE NATIONAL LABORATORY
Chemistry Division -03- (continued)

75. PHYSICAL AND SURFACE CHEMISTRY $400,000 03-3
D. M. Gruen, A. Krauss,
R. L. McBeth, M. Mendelsohn,
D. Steinbruchel, R. B. Wright,
M.-B. Liu

Experimental and theoretical studies of charge transfer processes at surfaces; excitation and deexcitation mechanisms of sputtered atoms, ions and molecules; effects on secondary ion fractions of monolayer coverages of oxygen on metals as monitored by simultaneous Auger analysis, energy and analyzed secondary ion mass spectroscopy and in situ XPS. Secondary photon and ion emission; determination of ionization coefficients at surfaces from measured energy distributions of secondary ions and neutrals; development of new techniques for measuring energy distributions of sputtered neutrals via Doppler shifted laser fluorescence spectroscopy; structural, compositional and other factors determining the thermodynamic stabilities of intermetallic hydrides; effects of the cubic to hexagonal transformation on the hydrogen sorption properties of AB_5 compounds; preparative methods for matrix isolated "naked" metal clusters and their cryochemistry; photochemistry of matrix isolated metal atoms and molecules of interest for catalysis.

76. HIGH-TEMPERATURE MATERIALS CHEMISTRY $436,000 03-3
R. J. Thorn, R. J. Ackermann,
G. E. Murch, E. G. Rauh,
W.-Y. Howng, G. H. Winslow,
J. Ziomek

High-temperature thermodynamic, transport and x-ray and electronic structural properties of inorganic, ceramic and metallic materials with special emphasis on the behavior of materials in energy systems such as LMFBR, HTGR, GCTBR, MHD and CTR; fundamental concepts of high-temperature chemistry in terms of lattice defects, phonon-electron interactions, and altered valent or aliovalent cations in nonstoichiometric phases; measurements of partial molar enthalpies and entropies of sublimation, phase equilibria, electronic structures with photoelectron spectroscopy, high-temperature x-ray diffraction and diffusion in uranium carbides and oxides; investigations of chemistry of condensation, especially of metastable phases and in relation to processes in energy systems; calculations related to defects and valence states through lattice potentials and ionic character of bonding. Monte Carlo evaluation of partition functions and computer simulation of diffusion in nonstoichiometric phases; studies of molecular ions present in thermal excursions in reactors; evaluation of thermochemical systematics and data of lanthandie and actinide phases; materials studied: oxides and carbides of uranium, rare-earth and actinide fluorides, β-aluminas, ZrO_2, Y_2O_3, ThO_2, $LaCrO_2$ with Mg and Sr, $Cs_2O.xSiO_2$, glasses and slags.

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

77. LIQUID METALS CHEMISTRY — $245,000 — 03-2
V. A. Maroni, E. Veleckis,
W. Calaway

Measurement of thermodynamic and transport properties of liquid alkali metals and their solutions; phase diagrams and solution thermodynamics of Li-Al-H, Li-Pb-H, Li-Si-H, and Ca-Ni-H systems by a tensimetric-titration method; solubilities of Li_2O and Li_2C_2 in liquid lithium; analysis of the chemical interactions in the lithium-carbon-nitrogen system; distribution of oxygen, nitrogen, and carbon between liquid lithium and selected austenitic and refractory alloys by resistivity techniques; surface interactions of lithium with refractory metals and alloys; corrosion mechanisms of refractory metals and alloys in liquid metals.

78. CHEMISTRY OF MATERIALS — $350,000 — 03-2
R. Kumar, B. Holt,
B. Hubble, H. R. Isaacson,
S. Johnson

Research on chemistry of sulfate and nitrate airborne particles and their formation mechanisms using stable isotope-ratio analysis; development of methodology and instrumentation for aerosol characterization as functions of size, time, and spatial variations by GC-FID methods and by Fourier-Transform infrared spectroscopy; study of kinetics of sulfur fixation by minerals (e.g., dolomite) and of the regeneration of active material from sulfated product with emphasis on mechanism of the reactions.

79. PHYSICAL CHEMISTRY OF ELECTRO-CHEMICAL SYSTEMS — $150,000 — 03-2
Z. Nagy, C. Melendres,
M. Blander, M. Saboungi

Electrochemical studies of processes occurring at cell electrodes and in electrolytes with emphasis on kinetics and mechanisms in the lithium aluminum/LiCl-KCl/metal sulfide cells and other electrochemical systems; study of metal (Fe, Co, Ni) and sulfide (FeS, NiS) dissolution/deposition reactions in molten salts by galvanostatic double-pulse and rotating-disc electrode techniques, respectively; thermodynamic measurements on lithium and sodium alloys emphasizing systems that show promise as battery electrodes (e.g., LiAlMg, LiMgCa); prediction of thermodynamic properties of ternary alloys and their phase diagrams using fundamental solution theories; extension of theories and experimental tests of extensions.

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

80. CALORIMETRIC STUDIES OF ENERGY RELATED MATERIALS — $130,000 — 03-2
C. E. Johnson, W. N. Hubbard
G. K. Johnson, K. Kim

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., benzofuran, thioxanthone, acridene, etc.) that are "building block molecules" of coal, and (2) compounds formed between glass systems (e.g., pollucite, scheelite) and actinides or fission products that are considered for storage of nuclear wastes; enthalpies of 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; measurement techniques include oxygen, fluorine, and hydrogen-bomb calorimetry, hypergolic and flow calorimetry, and drop calorimetry to 2000°C.

81. CHEMISTRY OF MOLTEN SALTS AND METALLURGICAL PROCESSES — $115,000 — 03-2
M. Blander, Z. Nagy,
M. Saboungi, J. Settle

Prediction of thermodynamic properties and phase diagrams of molten salts using fundamental solution theories; application of theories to silicates and to solutions containing acid salts; extension of theories and experimental tests of extensions; measurement of the solubilities of transition metal and heavy metal sulfides in molten salts; study of sulfide-polysulfide equilibria and complexing of cations by anionic species in molten salts. Research on fundamental chemistry of energy saving environmentally acceptable metallurgical processes; chemistry of aluminum electrowinning from cryolite and from chloride melts; interactions of Al^{+3} and $O^{=}$ ions in chloride melts; electro-dissolution of sulfide ores.

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

82. SURFACE, STRUCTURAL, AND MORPHOLOGICAL STUDIES ON ELECTROCHEMICAL STUDIES — $110,000 — 03-2
S. Siegel, C. Melendres, F. Cafasso

Studies at the submicroscopic and molecular levels of the various surface, structural, and morphological changes occurring during the operation of selected electrochemical systems; investigation of phenomena of electrocatalysis, electrode degradation, electrode wetting and dewetting, and dendrite growth; in-situ spectroscopic (Mossbauer and optical spectroscopy) and electrochemical investigations of electrocatalysis on model electrode/electrolyte systems; research on mechanisms of oxide/molten salt electrodes and of corrosion of metals in molten salts.

83. HEAT TRANSFER MATERIALS AND SALT VAPORS — $96,000 — 03-2
L. Curtiss, D. Frurip, M. Blander

Experimental and quantum mechanical studies on materials that exhibit strong or unusual bonding in the vapor and that may either have potential as heat-transfer fluids or can enhance gas phase mass transport; emphasis on the nature of vapor species, their equilibrium constants, their relative bond strengths and their structure; systems under investigation include trifluoroethanol pyridine, acetic acid, trifluoraecetic acid (TFA), binary mixtures of these compounds with water and high-temperature associated species formed between acid halides (e.g., BCl_3, $AlCl_3$) and bases (e.g., NH_3, Ch_3CN).

84. SEPARATIONS AND CATALYTIC PROCESSES — $40,000 — 03-2
G. Papatheodorou

Research on spectroscopic and thermodynamic properties of vapor and vapor complexes, some having potential in separation processes and other applications; study of high-temperature complexes of transition, lanthanide, and actinide halides with acidic gases (e.g., Al_2Cl_6, Fe_2Cl_6); identification and characterization of vapor species by Raman and resonance Raman spectroscopy coupled with systematization of the thermodynamics of formation of the complexes principally by electronic absorption spectroscopy; study of the mechanisms of hydrogenation of polycylic aromatic hydrocarbons in low melting acidic molten salts (e.g., $AlCl_3$, $InCl_3$, $SbCl_3$) by Resonance Raman spectroscopy; investigation of nature of organic radical cations formed in solution and of the effects of acid-base nature of the solvent and temperature on species, solvent-solute interactions, overall mechanism, and products, as part of the catalytic studies.

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

85. MHD SEED RECOVERY CHEMISTRY — $25,000 — 03-2
C. Johnson

Thermodynamic, kinetic, and computer modeling studies of reactions between potassium seed compounds and synthetic ceramic systems; effusion-mass spectrometric investigations of effects of additives on potassium activity in seed-slag systems and identification of species above the systems with emphasis on understanding interactions that may limit recovery of potassium seed from magnetohydrodynamic (MHD) systems.

86. MOLTEN SALT CHEMISTRY — $130,000 — 03-2
M. Blander, M. Saboungi,
G. Papatheodorou

This program includes (1) the investigation on the applicability of fundamental solution theories in the calculation of phase diagrams and other thermodynamic properties of molten salts, and (2) the study of thermodynamics and structure of high-temperature associated species formed between acid halides (e.g., BCl_3) and bases (e.g., NH_3). To be phased out in FY 1979.

87. BONDING AND STABILITY OF SULFUR DIOXIDE SORBENT MATERIALS — $30,000 — 03-2
S. Siegel

Research on the bonding factors that govern decrepitation of dolomite and calcite stones--a phenomenon found to occur in fluidized beds when these stones are used as sulfur dioxide sorbents. This program is now terminated.

BROOKHAVEN NATIONAL LABORATORY
Upton, Long Island, New York 11973

Corrosion Science Group -01-
D. H. Gurinsky - Phone: (FTS) 664-3504 or 516-345-3504
W. Y. Kato - Phone: (FTS) 664-2444 or 516-345-2444
J. R. Weeks - Phone: (FTS) 664-4617 or 516-345-2617

88. INTERGRANULAR STRESS CORROSION $190,000 01-2
J. R. Weeks, Brihesh Vyas,
M. W. Kendig, Y. S. Park,
M. Suenaga, A. H. Winter

Electrochemistry of surfaces of iron and nickel base alloys under stress as revealed by scanning reference electrode and ac polarization techniques. Determination of sensitization of stainless steel using these techniques. Measurements of chromium depletion and grain boundary segregation in stainless steels and Inconel 600 using energy dispersive x-ray analysis attached to a transmission electron microscope. Measurements of the strain rate dependence of the stress corrosion of sensitized stainless steels and Inconel 600 in high temperature water.

Materials Science Division -01-
D. H. Gurinsky - Phone: (FTS) 664-3504 or 516-345-3504
M. Suenaga - Phone: (FTS) 664-4518 or 516-345-3518

89. RELATIONSHIP BETWEEN PROPERTIES AND STRUCTURES $650,000 01-3
R. Caton, D. Dew-Hughes,
O. F. Kamerer, K. Lee,
C. Pande, M. Suenaga, D. O. Welch

Fundamental properties of high critical temperature superconductors; order parameter, phase stability, stoichiometry, heat capacity measurements, neutron irradiation, x-ray and neutron diffraction, and normal state resistivity: Preparation of high critical field, high critical current and critical temperature superconductors: Kinetics and mechanism of A15 superconductor formation in solid state diffusion process: Mechanical deformation process in A15 superconductors: Hydrogen embrittlement and hydrogen attack in Fe and steels: Use of small angle neutron scattering for examination of materials.

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

90. BASIC PROCESSES AND STRUCTURAL PROPERTIES OF AMORPHOUS SEMICONDUCTOR THIN FILMS FOR SOLAR ENERGY CONVERSION — $0 — 01-3
R. W. Griffith, F. Kampas, P. Vanier

Fundamental materials investigations on the electrical, optical, and microstructural properties of amorphous semiconductor thin films that are tailored for efficient solar energy conversion. The basic nature of localized states contained in the mobility gap 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 and hydrogenation of semiconductor films.

91. PHYSICAL METALLURGY OF METAL HYDRIDE SYSTEMS — $100,000 — 01-3
D. Dew-Hughes, M. Pick, D. O. Welch

Studies of the metallurgical factors which influence the hydriding behavior of certain metal systems of hydrogen in metals and alloys: Potential metal hydrogen systems as hydrogen storage media such as FeTi, NiTi, CoTi, etc: Influence of substitutional atoms in Nb on hydriding behavior and of crystalline structures on hysteresis: Effects of surface contamination of hydriding process: Techniques of EXAF, TEM, neutron diffraction are used.

92. RADIATION DAMAGE — $200,000 — 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: voids and gases in metals.

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

93. EFFECT OF MICROSTRUCTURE AND ENVIRONMENT UPON FRACTURE TOUGHNESS — $100,000 — 01-2
A. Arbel, D. Dew-Hughes

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.

Physics Department -02-
M. Blume - Phone: (FTS) 664-3745 or 516-345-3735

94. NEUTRON SCATTERING - MAGNETIC SYSTEMS — $571,000 — 02-1
S. M. Shapiro, J. D. Axe,
L. Passell, G. Shirane,
J. A. Tarvin, W. Thomlinson

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.

95. NEUTRON SCATTERING - PHASE TRANSITIONS — $617,000 — 02-1
G. Shirane, J. D. Axe, J. Eckert,
W. D. Ellenson, Y. Noda, S. M. Shapiro,
R. Youngblood, R. Currat

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.

96. NEUTRON SCATTERING - ELEMENTARY EXCITATIONS IN SOLIDS — $548,000 — 02-1
J. D. Axe, J. Eckert, W. D. Ellenson,
L. Passell, S. M. Shapiro, G. Shirane,
W. Thomlinson

Neutron spectrosocpy of low-lying excited states in solids; electron-phonon interactions in metals; dynamics of mixed valence systems; lattice dynamics of high pressure phases of solid ^{4}He; anharmonic phonon effects in perovskites.

BROOKHAVEN NATIONAL LABORATORY
Physics Department -02- (Continued)

97. NEUTRON SCATTERING - PARTIALLY ORDERED SYSTEMS — $549,000 — 02-1
L. Passell, S. M. Shapiro, J. Eckert, W. D. Ellenson, J. A. Tarvin, W. Thomlinson

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 ^4He films adsorbed on graphite.

98. EXPERIMENTAL RESEARCH - SPECTROSCOPY OF SOLIDS — $193,000 — 02-2
B. C. Frazer and J. B. Hastings

X-ray and neutron studies of structural, dynamic and electronic properties of solids. Diffuse scattering in ferroelectric phase transitions. Central peak enhancement due to defects in $SrTiO_3$. EXAFS studies with synchrotron radiation: dilute alloys with Fe in Cu and V, and Ti in Fe; structural changes in the KH_2AsO_4 phase transition.

99. EXPERIMENTAL RESEARCH - NATIONAL SYNCHROTRON LIGHT SOURCE — $622,000 — 02-2
A. van Steenbergen, B. C. Frazer, J. Godel, M. Perlman, K. Batchelor, J. Bittner, L. Blumberg, B. Culwick, J. Galayda, J. B. Hastings, R. Heese, M. Howells, H. Hsieh, S. Krinsky, J. Sheehan, J. Schuchman, R. Watson

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
Physics Department -02- (Continued)

100. THEORETICAL PHYSICS — $505,000 — 02-2
V. J. Emery, J. Black, M. Blume, G. J. Dienes, J. Fields, R. H. Swendsen, R. E. Watson, S. Aubry (C.E.N., Saclay), B. L. Gyorffy

Phase transitions and critical phenomena, magnetism, liquid helium (He-3, He-4, and their mixtures), ferroelectricity, electronic structure of metals and alloys, and crystal defect physics; properties of one- and two-dimensional materials, crystal growth and adsorbed films on surfaces; computer studies of one- and two-dimensional systems and random magnetic systems; commensurate-incommensurate phase transitions, analysis of soft x-ray photoemission data from alloys; properties of disordered materials; defect-defect interactions; molecular dynamical calculations of equations of state and shock waves; studies of valence electron distributions in crystals.

101. PARTICLE-SOLID INTERACTIONS - RADIATION EFFECTS RESEARCH — $373,000 — 02-4
A. N. Goland, P. W. Levy, K. G. Lynn, Y. Platov

Studies of neutron- and electron-irradiated metals and alloys employing positron-annihilation lifetime and Doppler-broadening measurements as well as electrical resistivity studies; simultaneous optical absorption and luminescence measurements during electron irradiation of ceramics, glasses, alkali halides and minerals, diagnostic calculations of high-energy neutron damage with emphasis on fusion reactor materials including nonmetals.

102. PARTICLE-SOLID INTERACTIONS - PROPERTIES OF REAL SOLIDS — $426,000 — 02-4
K. G. Lynn, P. W. Levy, J. E. Dickman, A. N. Goland

Utilization of particle-solid interactions as diagnostic probes in solid-state physics investigations; electron states in solids by positron-annihilation measurements, development of slow-positron beam for surface studies; investigation of point defects and dislocations in annealed and deformed metals by positron-annihilation lifetime and Doppler broadening measurements; applications of μ+SR to defect problems in solids; geophysics of mineral thermoluminescence.

BROOKHAVEN NATIONAL LABORATORY
Physics Department -02- (Continued)

103. PARTICLE-SOLID INTERACTIONS - ADVANCED MATERIALS SYNTHESIS AND CHARACTERIZATION — $160,000 — 02-4
D. E. Cox, A. Moodenbaugh, B. C. Frazer

Solid electrolytes, electrode materials for MHD power generation, structural disorder and other defects in superconductors. Preparation and characterization of high temperature oxide systems based upon La_2O_3; defect fluorite structure analysis, high-T_c superconductor studies.

104. PARTICLE-SOLID INTERACTIONS - ALTERATION AND ANALYSIS OF SOLIDS BY ION BEAMS — $106,000 — 02-4
A. N. Goland, J. S. Rosner, M. Strongin

High resolution Rutherford backscattering for materials analysis, materials modification by ion implantation, channeling phenomena in thin single crystals, charge-states of channeled heavy ions, ion-induced lattice damage and studies of the relationship between defect structure and superconducting properties of thin-film A-15 superconductors.

105. ENGINEERING PHYSICS - SUPERCONDUCTIVITY — $398,000 — 02-5
A. Ghosh, H. Lutz, M. Strongin

Superconductivity and transport properties in A-15 films; studies of "saturation" of resistance at high temperatures and anomalous temperature dependence of the resistivity of low temperatures; studies of the density of states in disordered A-15's; investigations of resistivity, density of states, and T_c changes with disorder in low T_c A-15's such as Mo_3Ge. Transport measurements in highly disordered and amorphous materials. Photoconductivity and electrical conductivity measurements on hydrogenated amorphous silicon; new techniques for making hydrogenated a-silicon.

BROOKHAVEN NATIONAL LABORATORY
Physics Department -02- (Continued

106. ENGINEERING PHYSICS - SURFACE STUDIES — $132,000 — 02-5
R. J. Smith, M. Strongin, J. Strozier, M. Yu

Use of photoemission with polarized radiation to determine orientation and geometry of adsorbates chemisorbed on transition metals; studies of electronic properties of clean surfaces. The physics of secondary ion mass spectroscopy and applications to chemisorption; correlation with chemisorption bands and surface phases. Use of a.c. pulsing techniques under ultra-high vacuum conditions to study chemical reactions at surfaces.

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

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

107. WELDING RESEARCH $180,000 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; grain boundary characterization influence of oxygen and trace elements in the embrittlement process.

108. GEOTHERMAL SCALING AND CORROSION RESEARCH $130,000 03-3
L. A. Casper, W. F. Downs

Chemical mechanisms of scaling and corrosion; dissolution kinetics and thermodynamics of calcium carbonate polymorphs in synthetic geothermal solutions; rotated ring disk electrode apparatus to determine the chemical kinetics of mass transfer at a heat exchanger surface; mapping of the chemistry of metal surfaces to determine sites which promote nucleation of scale components or the initiation of corrosion.

ILLINOIS, UNIVERSITY OF
Urbana, Illinois 61801

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

109. LOCALIZED CORROSION OF PASSIVE METALS — $ 40,000 — 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.

110. MECHANISMS OF STRESS-CORROSION CRACKING — $ 84,000 — 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.

111. CHARACTERIZATION OF COMPOUNDS AND ALLOYS — $126,000 — 01-1
H. L. Fraser, C. A. Wert

Development of microchemical and analytical methods on 20 Å scale using electron energy loss and energy dispersive spectroscopies. Application to hydride and carbide precipitate formation in bcc metals, to oxide and semiconducting compounds, and to microcharacterization of coal.

112. HYDROGEN BEHAVIOR IN BCC METALS — $140,000 — 01-3
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.

113. DYNAMICAL STRUCTURE OF MATERIALS UNDER EXTREME CONDITIONS OF TEMPERATURE AND PRESSURE — $125,000 — 01-1
J. Jonas

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

ILLINOIS, UNIVERSITY
Materials Research Laboratory -02- (Continued)

114. THEORY OF POLYMERS — $ 15,000 — 01-1
R. J. Gaylord

Morphology of chain confinement in semicrystalline polymers, block copolymers and filled elastomers; effect on deformation and anelasticity.

115. SOLID DIELECTRICS — $ 49,000 — 01-3
D. A. Payne, W. Petusky

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.

116. PHYSICAL PROPERTIES OF OXIDE CERAMICS — $ 36,000 — 01-3
G. P. Wirtz

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

117. SITE LOCATIONS IN CERAMIC MATERIALS — $ 63,000 — 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 methods.

118. MECHANICAL PROPERTIES OF MATERIALS — $ 43,000 — 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.

119. ELECTRONIC PROPERTIES OF ORGANIC SEMICONDUCTORS — $ 49,000 — 01-3
T. J. Rowland

Electrical, magnetic and magnetic resonance investigation of doped one-dimensional organic semiconductors.

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory -02- (Continued)

120. LOW TEMPERATURE STUDIES OF DEFECT STRUCTURE IN SOLIDS — $100,000 — 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.

121. RESPONSE OF SOLIDS TO ELECTROMAGNETIC RADIATION — $ 31,000 — 02-2
J. D. Dow

Optical semiconductor response to intense light; deep trap efficiencies in model photovoltaic and electroluminescent materials. LEED and photoelectron spectra of layered dichalcogenides. Theory of synchrotron radiation spectra of deep cores in metals.

122. USE OF VERY HIGH PRESSURES TO INVESTIGATE THE STRUCTURE OF MATTER — $118,000 — 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 related properties of polymer solutions.

123. IMPURITIES IN SUPERCONDUCTORS — $ 43,000 — 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.

124. ULTRASONIC INVESTIGATIONS OF THE STRUCTURE OF MATTER — $125,000 — 02-2
A. V. Granato

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

125. PROPERTIES OF CRYSTALLINE CONDENSED GASES — $ 95,000 — 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.

ILLINOIS, UNIVERSITY
Materials Research Laboratory -02- (Continued)

126. DEFECT PROPERTIES OF SOLIDS — $161,000 — 02-2
D. Lazarus

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

127. NUCLEAR MAGNETIC RESONANCE IN SOLIDS — $130,000 — 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.

128. PHYSICAL PROPERTIES OF TRANSITION METAL CARBIDES — $ 77,000 — 02-2
W. S. Williams

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

129. RADIATION DAMAGE IN SOLIDS — $140,000 — 02-4
J. S. Koehler

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

LAWRENCE BERKELEY LABORATORY
University of California
Berkeley, California 94720

Materials and Molecular Research Division
D. A. Shirley - Phone: (FTS) 451-5619 or 415-843-2740

130. MICROSTRUCTURE, PROPERTIES AND ALLOY DESIGN - ELECTRON DIFFRACTION AND MICROSCOPY — $350,000 — 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 and diffraction and high voltage electron microscopy.

131. 1.5 MeV ELECTRON MICROSCOPE — $100,000 — 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 contaminating or hostile environments.

132. POWDER METALLURGY — $100,000 — 01-1
M. Pickus

Application of fundamental principles of materials science and high temperature chemistry to the design of new materials required in advanced technologies, and to the development of special processing techniques for obtaining them in useful forms. Multiphase composites of brittle intermetallic compounds in metallic matrices for application in severe environments, and rare-earth containing intermetallic compounds with useful magnetic properties. Use of a low melting additive which provides a transient liquid during the sintering cycle; microstructure control of liquid phase sintered iron-carbon alloys; preparation of powders with metastable structures.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

133. ATOMIC RESOLUTION MICROSCOPY — $0 — 01-1
R. Gronsky, G. Thomas

Development and use of the most sophisticated electron imaging techniques to photograph atoms in crystalline or amorphous arrangements and provide for real-space structural analysis. Localized atomic configurations responsible for solid state reactions, bulk as well as surface properties, and material failure in new energy technologies. To be initiated in FY 1979.

134. THEORETICAL PROBLEMS IN ALLOY DESIGN — $345,000 — 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.

135. RELATIONS BETWEEN DISLOCATIONS, POINT DEFECTS, AND PROPERTIES OF METALS — $225,000 — 01-2
J. Washburn

Structural characterization and measurement of properties of materials potentially useful to collection, conversion and storage of solar energy. Point defect clustering, properties of grain boundaries and mechanisms of mass transport in amorphous silicon; high resolution transmission electron microscopy. Transport properties of mixed cadmium-zinc sulfide single-crystal layers. Growth of zinc diphosphide as a possible new material for solar cell use. Size distribution of particles in spectrally selective electroplated black chrome surface layers for high absorption in the visible and low emissivity in the far infrared.

136. HIGH TEMPERATURE OXIDATION AND CORROSION OF MATERIALS — $160,000 — 01-2
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.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

137. SUPERCONDUCTIVITY EFFECTS - HIGH FIELD SUPERCONDUCTIVITY — $220,000 — 01-3
M. Pickus

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 emphasizes 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.

138. MICROSTRUCTURE AND MECHANICAL BEHAVIOR OF CERAMIC MATERIALS; GLASS AND CERAMIC-METAL SYSTEMS — $195,000 — 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 constituents are within the Al_2O_3-SiO_2 system. Thermodynamic considerations of sintering with and without a liquid phase. Relationship of 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.

139. HIGH TEMPERATURE REACTIONS — $235,000 — 01-3
A. W. Searcy

Transport kinetics of vapor mixtures through porous solids. Kinetics of decomposition of strontium carbonate. Catalysis of the decomposition of strontium sulfate. The effects of temperature, CO_2 pressure, and particle size on the surface area of calcium oxide formed by decomposition of calcite. Variation of thermodynamic stability and surface area of magnesium hydroxide. Catalysis of the sintering of calcium oxide by carbon dioxide. Solution thermodynamics of solid calcium carbonate. Theoretical studies on the kinetics of decomposition reactions and on surface thermodynamics.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

140. RELATION OF MICROSTRUCTURE TO PROPERTIES IN CERAMICS — $195,000 — 01-3
J. A. Pask, A. W. Searcy

Microstructure and properties of ceramic materials. Densification of powder compacts with and without a liquid phase; use of a hot stage scanning electron microscope facility developed for this purpose. Densification and grain growth kinetics; effect of ambient atmosphere. Piezoelectric and ferroelectric properties in ceramic materials. Thick film conducting systems on ceramic substrates. Bonding microstructure in the metallic phase, reduce precious metal contents.

141. 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 1000°C - 3000°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. Composites: 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.

142. MECHANICAL PROPERTIES OF CERAMICS — $0 — 01-3
A. G. Evans

Study of concurrent deformation and fracture processes in ceramics polycrystals at elevated temperatures to evolve schemes for characterizing and predicting high temperature failure. Microstructural causes of toughening, investigation of crack tip process zones at high resolution. Development of a quantitative framework for the design of microstructures for ceramics. Erosion-Corrosion phenomena in ceramics, toughness and hardness properties of corrosion layers. To be initiated in FY 1979.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

143. EROSION-CORROSION-WEAR PROGRAM — $430,000 — 01-5
A. V. Levy

Determination of solid particle erosion and combined erosion-corrosion mechanisms. Surface chemistry of hot combined, reactive, flowing gases and char particle in contact with metals and ceramics of different compositions. Mechanisms of formation, composition, morphology and behavior of surface scales; protective barriers.

144. IN-SITU INVESTIGATION OF GAS-SOLID REACTIONS BY ELECTRON MICROSCOPY — $0 — 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. To be initiated in FY 1979.

145. EXPERIMENTAL SOLID STATE PHYSICS AND QUANTUM ELECTRONICS — $205,000 — 02-2
Y. 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.

146. FAR INFRARED SPECTROSCOPY — $170,000 — 02-2
P. L. Richards

Development of improved types of far infrared detectors, mixers and spectrometers. Use of advanced infrared techniques for measurement of: the infrared radiation left over from the creation of the universe, radiation from dust clouds in our galaxy, infrared spectra of impurities in semiconductors, far infrared spectra of electrons trapped on the surface of liquid helium and near infrared absorption spectra of molecules chamically adsorbed on metal surfaces.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

147. EXCITED QUANTUM FLUIDS IN SOLIDS — $125,000 — 02-2
C. 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 diagram; 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.

148. SUPERCONDUCTIVITY, SUPERCONDUCTING DEVICES, AND 1/f NOISE — $200,000 — 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.

149. THEORETICAL SOLID STATE PHYSICS — $ 60,000 — 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 non-phonon mechanisms for superconductivity and properties of high transition temperature A15 superconductors; development of pseudopotential theory.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

150. LOW TEMPERATURE PROPERTIES OF MATERIALS — $115,000 — 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. Establishment of a temperature scale for the region from 0.06 to 25K based 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.

151. HIGH PRESSURE CHEMISTRY — $ 40,000 — 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 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.

152. ELECTROCHEMICAL PROCESSES — $115,000 — 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 macro-profiles. 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.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

153. HIGH TEMPERATURE THERMODYNAMICS — $100,000 — 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.

154. CHEMISTRY AND MATERIALS PROBLEMS IN ENERGY PRODUCTION TECHNOLOGIES — $145,000 — 03-3
D. 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.

155. ELECTROCHEMICAL PHASE BOUNDARIES — $135,000 — 03-3
R. H. Muller

Investigation of new means to accelerate electrochemical mass transport in order to increase the space-time yield and energy efficiency of electrochemical processes. Formation of boundary layers and thin films at electrochemical interfaces. Development and use of new optical techniques in combination with simultaneous electrical measurements and selected methods of contemporary surface science.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

156. SOLID STATE AND SURFACE REACTION — $280,000 — 03-3
G. 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.

157. NUCLEAR MAGNETIC RESONANCE — $120,000 — 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.

158. PLASMA ENHANCED DEPOSITION OF THIN FILMS — $0 — 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. To be initiated in FY 1979.

LAWRENCE LIVERMORE LABORATORY
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

159. HOT CORROSION STUDIES RELATED TO FOSSIL FUELS — $180,000 — 01-1
D. W. Short, 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 sutdied by weight change and scale growth; salt-substrate interactions; molten salt electrochemical reactions; effects of oxide additions to a given salt.

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

Selection, preparation and preliminary screening of amorphous alloys based on quenching by ejecting molten metal in a continuous stream from a nozzle against a spinning cylinder; sputtering technique also used for preparation of alloys; X-ray diffraction and differential scanning calorimetry.

161. LOW INDEX OPTICAL MATERIALS RESEARCH — $216,000 — 02-2
J. J. Weber, C. Cline, W. L. Smith, D. Milam

Nonlinear optical properties of materials subjected to intense light beams; intensity-dependent refractive index change and multiphoton absorption; optical materials studies include: glasses (BeF_2), crystals (alkali halides, fluorides, oxides), and polymers; time-resolved interferometry used to measure nonlinear refractive index.

162. OPTICALLY-INDUCED DAMAGE IN TRANSPARENT DIELECTRIC MATERIALS — $ 88,000 — 02-2
D. Milam, W. L. Smith, M. J. Weber

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 fluoride crystals; and thin films; studies of electron avalanche, multiphoton absorption, bulk absorption, surface properties, and nonlinear absorption.

LAWRENCE LIVERMORE LABORATORY (Continued)

163. LASER-EXCITED FLUORESCENCE IN AMORPHOUS SOLIDS — $ 90,000 — 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.

164. THIN FILM MATERIALS STUDIES FOR LASER OPTICAL COATINGS — $216,000 — 02-2
J. Khan

To develop a quantitative understanding of the factors that influence the properties of thin films; 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.

165. D_2-DT-T_2 PHASE DIAGRAM — $140,000 — 03-2
C. Souers

To measure deviations from Raoult's Law of D-T mixtures-solid and liquid; to determine the extent of fractionation in large frozen samples; to determine the kinetics of chemical and ortho-para reactions. Infra-red spectroscopy will be developed as new quantitative tool for the study of liquid and solid D-T. Methods for separating pure molecular DT will be investigated.

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

Chemistry - Materials Science Division
R. D. Baker - Phone: (FTS) 843-4563 or 505-667-4563
M. G. Bowman - Phone: (FTS) 843-6014 or 505-667-6014

166. HIGH TEMPERATURE MATERIALS FOR ENERGY APPLICATIONS — $210,000 — 01-2
E. K. Storms, B. A. Mueller, D. L. Rohr

Knudsen and Langmuir vaporization of various compositions near LaB_6; boron and lathanum 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.

167. HIGH TEMPERATURE IRRADIATION DAMAGE STUDIES — $300,000 — 01-4
J. R. Cost, W. V. Green, L. S. Levinson, D. M. Parkin, W. F. Sommer

Proton irradiation with LAMPF beam; concurrent cyclic stressing; dislocation vibration; void growth; numerical analysis of point defect diffusion during pulsed irradiation; dislocation damping measurements of interstitial escaping cascades, during electron, neutron and proton irradiation; search for point defects in irradiated amorphus metals.

168. MATERIAL DEFORMATION UNDER MULTI-AXIAL LOADING — $70,000 — 01-5
S. S. Hecker, J. J. Petrovic

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

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

Simultaneous measurement of diffusion coefficient and solubility of hydrogen isotopes (including tritium) in liquid lithium and container materials Nb, Nb-1%Zr, Ni, Fe-2 1/4% Cr - 1% Mo over the temperature range 1000-1400K and a pressure range 10^2 - 10^4 Pa; incorporation of the results into theories of diffusion in liquids; development of an infusion technique which allows for Sieverts' law behavior of hydrogen isotopes in metals; determination of the effect of impurities and radiation damage on transport properties; measurements of phase diagrams and isotope effects in appropriate metal-tritium and alloy-tritium systems; removal of tritium from helium streams using eutectic alloys.

Energy/Q Division
W. E. Keller

170. ULTRAHIGH PRESSURE STUDIES OF HYDROGEN — $120,000 — 02-2
R. L. Miller

Adaptation of diamond-anvil cells for experiments on cryogenic gases to 200 k bar; measurements of pressure, volume, temperature, and ultrasonic velocity; work on a two stage system combining the piston-cylinder and diamond anvil techniques to pressurize hydrogen to 1 M bar.

Theoretical Division
P. Carruthers

171. LOS ALAMOS EQUATION OF STATE LIBRARY — $200,000 — 02-3
B. I. Bennett

Maintain file of materials properties which can be accessed by computer codes in a variety of applications; used for realistic hydrodynamics calculations; continuing effort to develop and improve theoretical models.

LOS ALAMOS SCIENTIFIC LABORATORY
Theoretical Division (continued)

172. ELASTIC WAVE SCATTERING AND QUANTITATIVE FLAW IDENTIFICATION — $100,000 — 01-5
J. E. Gubernatis

Development of an analytical scientific reference data base for flaw identification; calculations of scattering phenomena selected as representative of applications; study will use principally an integral equation to describe the scattering permitting a systematic development of approximations; scattering will be calculated for special geometries by various approximations and compared with exact results from a sphere.

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

173. HIGH TEMPERATURE FLUIDS FOR ENERGY SYSTEMS — $220,000 — 01-3
L. J. Wittenberg

Characterization at elevated temperatures of potentially useful liquid systems for advanced energy concepts; fluids for solar photothermal absorption processes and electrotransport of tritium in liquid lithium; identification of soluble chromophoric materials dissolved in fluids which are liquids at ambient temperatures; absorptivities, emissivities, long-term thermal stability.

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

Metals and Ceramics Division -01-
J. R. Weir, Jr. - Phone: (FTS) 850-1554 or 615-483-1554
C. J. McHargue - Phone: (FTS) 850-1277 or 615-483-1277

174. THEORETICAL STUDIES OF METALS AND ALLOYS — $380,000 — 01-1
J. S. Faulkner, W. H. Butler
G. S. Painter, G. M. Stocks,
M. H. Yoo

Interstitial dislocation loop nucleation and growth during charged particle irradiation, role of self-ion deposition, cascades, and solute trapping; CPA treatment of electronic states in random alloys (Cu-Ni, Cu-Zn, Cu-Al, Nb-Mo); layer and cluster calculations for surfaces, O and CO chemisorbed on Cu, O on Al; superconducting transition temperature and phonon linewidth in Nb; contribution of lattice conduction to thermal conductivity in metals and alloys; calculation of binding energies in solids.

175. X-RAY SCATTERING RESEARCH — $235,000 — 01-1
H. L. Yakel, B. S. Borie,
R. W. Hendricks, J. S. Lin,
C. J. Sparks

Small angle x-ray scattering sutides of voids and loops in irradiated metals, porosity in coals, poisoning of catalysts, and structure of polymers; crystallography of modulated structures and defect structure of FeS; theoretical and experimental studies of extinction phenomena; inelastic resonance scattering.

176. PREPARATION AND SYNTHESIS OF HIGH TEMPERATURE MATERIALS — $310,000 — 01-1
G. W. Clark, S. L. Bennett,
C. B. Finch, J. D. Holder,
C. F. Yen

Directional solidification of binary and ternary metal-non-metal systems (oxides, carbides, borides, nitrides); 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) for tool applications; theoretical treatment of coupled solidification and the IZG (internal zone growth) and EFG (edge-defined film-fed growth) processes; actinide-doped halide crystals; hydrothermal growth of quartz and II-IV compounds.

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

177. EROSION AND WEAR OF CERAMICS — $300,000 — 01-1
C. S. Yust, C. F. Yen

TEM and SEM studies of damage by multi-particle impact on polycrystalline mullite and alumina to 470°C; subsurface structure of single particle damage in single crystal alumina, friction and microstructural changes caused by sliding wear, effect of temperature, atmosphere, crystal orientation; strength and deformation mechanisms in ceramics.

178. STRUCTURE OF COAL — $85,000 — 01-1
L. A. Harris, C. S. Yust

TEM, SEM, microprobe, optical and infrared petrography studies of microporosity and micromineralogy of specific macerals in coals.

179. X-RAY RESEARCH USING SYNCHROTRON — $80,000 — 01-1
C. J. Sparks, H. L. Yakel

Development and application of techniques using the x-rays at Stanford Synchrotron Radiation Laboratory; fluorescence experiments for trace elements and low concentrations of defects and surface layers; search for short- or long-range chemical order in Fe-Ni-Cr steels, sigma phase and mixed oxide phases.

180. HIGH VOLTAGE AND ANALYTICAL ELECTRON — $300,000 — 01-1
R. W. Carpenter, J. Bentley,
E. A. Kenik, N. Zaluzec

Development and application of analytical transmission electron microscopy and high voltage electron microscopy to determine the microstructure and microchemistry of solids; weak-beam dark field studies of precipitates in neutron irradiated alloys; SAES of internally oxidized Ta-W-Hf alloys; in-situ studies in the 1 MeV microscope using an environmental stage with heating and strain capabilities.

181. DEFORMATION AND MECHANICAL BEHAVIOR OF STRUCTURAL MATERIALS — $450,000 — 01-2
R. A. Vandermeer, J. C. Ogle,
T. C. Reiley, C. L. White

Relationships between structure, deformation mechanisms, and mechanical properties; rolling and recrystallization textures in Ta single crystals; annealing of voids; deformation modes, transformation and the shape-memory effects; grain boundary segregation and fracture in Fe-3% Si bicrystals; segregation to surfaces of creep voids; creep studies at strain rates of 5×10^{-10} sec^{-1}.

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

182. KINETICS AND MECHANISMS OF SURFACE AND SOLID STATE REACTIONS — $600,000 — 01-3
J. V. Cathcart, P. T. Carlson, R. E. Druschel, R. A. McKee, R. E. Pawel, G. F. Petersen

Defect interaction 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, Hall effect determination of mobile species; diffusion mechanisms and solute-lattice interactions for interstitial diffusion in oxides (T in TiO_2, Al_2O_3, Cr_2O_3, CoO); aliovalent impurity diffusion in oxides; fast diffusion in lead alloys; theoretical model for oxidation of zirconium alloys.

183. PHYSICAL PROPERTIES RESEARCH — $300,000 — 01-3
D. L. McElroy, J. P. Moore, R. K. Williams, R. O. A. Hall

Development and application of measurement methods for physical property studies from 4.2 to 2600 K; lattice conduction and Lorenz function in Ni and Cr alloys; electron-phonon scattering in transition metals; Ettingshausen-Nernst effect in Ni alloys; thermal conduction in insulators; absorptivity and emissivity in thin films.

184. METALLURGY OF SUPERCONDUCTING MATERIALS — $300,000 — 01-3
C. C. Koch, A. DasGupta, D. S. Easton, D. M. Kroeger, W. Specking

Flux pinning in Nb bicrystals, calculations of pinning force in Hf-Nb and Ta-Nb alloys; stress effects on superconducting parameters in Nb_3Sn and V_3Ga; ac loss mechanism; preparation and properties of $PbMo_6S_8$; amorphous, microcrystalline and metastable phases.

185. RADIATION EFFECTS — $1,100,000 — 01-4
J. O. Stiegler, K. Farrell, J. Bentley, R. W. Carpenter, W. A. Coghlan, E. A. Kenik, M. B. Lewis, L. K. Mansur, N. H. Packan, T. C. Reiley, H. Schroeder

Analysis of neutron damage in aluminum-base binary alloys with respect to effect on void nucleation and growth; neutron damage in Zr, Ni, and Fe-Cr-Ni alloys; damage simulation studies using multiple ion beams from two accelerators, relationships between neutron and ion damage, role of gases in nucleation and growth of voids and interstitial loops; irradiation creep simulation using ORIC and neutron pre-irradiated specimens; phase stability during irradiation; theoretical analysis of void and loop growth, solute-defect interactions, and irradiation creep; HVEM irradiations.

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

186. FUNDAMENTAL STUDIES IN WELDING $250,000 01-5
G. M. Goodwin, S. David,
J. M. Leitnaker

Control of weld microstructure; effect of process parameters; heat and mass transport during solidification; composition, distribution, and stabilities of microphases; austenitic and ferritic steels.

187. STUDIES IN NONDESTRUCTIVE EVALUATION $0 01-5
R. W. McClung

Theoretical and experimental study of wave system resulting from interaction of an ultrasound wave with various kinds of internal boundaries in metals; effect of acoustic properties of the solid. To start in FY 1979.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-
M. K. Wilkinson - Phone (FTS) 850-6713 or 615-483-6713
F. W. Young, Jr. - Phone (FTS) 850-1704 or 615-483-6713

188. ELEMENTARY EXCITATIONS IN CONDENSED MATTER — $645,000 — 02-1
R. M. Nicklow, B. Alefeld
R. L. Cappelletti, W. P. Crummett,
W. C. Koehler, N. Kunitomi,
W. Lovesey, H. Miwa,
H. A. Mook, Y. Nakai,
H. G. Smith, Y. Tsunoda
L. Van Bodegom, N. Wakabayashi

Inelastic neutron scattering studies of phonons, magons, and single particle excitations in solids and liquids; lattice dynamics and molecular reorientation in NaO_2, lattice dynamics and crystal field excitations in γ-Ce, SmS and $Sm_xY_{1-x}S$, phonons and magnons in Ni-Pt, Fe-Pt, and Fe-V alloys, spin wave spectra in Pd(5% Fe), spin waves in amorphous Fe and Co, phonon measurements and phase transitions in TTF-TCNQ, $MEM(TCNQ)_2$, $TiSe_2$, and $Pd_{1-x}Ge_xTe$.

189. MAGNETIC PROPERTIES OF SOLIDS — $530,000 — 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 alloy systems Ni-Pt, Pd-Gd; magnetic structure of TmS; magnetic form factor and magnetic moment density in valence fluctuation systems SmS, $Sm_{.76}Y_{.24}S$, SmB_6, and $Ce_{.74}Th_{.26}$; induced moment form factor and moment density of Zr, dilute Fe-Cu alloys (Kondo systems), $CeSn_3$; magnon spectra and magnetic exchange in rare earth-Y alloys and Laves phase intermetallic compounds; magnetic short range order in Gd.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

190. PROPERTIES OF DEFECTS, SUPERCONDUCTORS, AND HYDRIDES — $525,000 — 02-1
W. C. Koehler, H. R. Child,
D. K. Christen, H. A. Mook,
R. M. Moon, F. Mueller
R. M. Nicklow, H. G. Smith,
S. Spooner, N. Wakabayashi

Elastic, inelastic, and small angle scattering of neutrons by superconductors, superionic conductors, metal hydrides, and by elements and compounds containing defects; high resolution neutron spectrometry of KCl(CN); phonon spectra of superconductors, α-U, Mo-Re, Al-15 type compounds; dynamic properties of tritium in metal systems; electron-phonon interactions in Nb and Mo; phase transitions in ^{7}LiD; phonon densities of states, magnetic structures, and crystal field excitations in reentrant superconductors; localized modes in Th(.06C); lattice dynamics and diffusive motion in silver halides; small-angle neutron scattering studies of void sizes and shapes in irradiated steel, Al, Nb; high resolution small-angle diffraction studies of fluxoid lattice morphology and anisotropy in high T_c superconductors.

191. PHYSICAL PROPERTIES OF SUPERCONDUCTORS — $405,000 — 02-2
S. T. Sekula, B. R. Appleton,
D. K. Christen, H. R. Kerchner,
R. H. Kernohan, O. A. Pringle
H. G. Smith, J. R. Thompson

Studies of fluxoid arrays, flux flow, flux creep, fluxoid-defect interactions, and anisotropy in Nb-, V-, and Ta-base alloys and superconducting compounds (A15 and B1); dc magnetization, ac magnetic permeability, critical currents, and normal-state electrical transport; small-angle neutron scattering by fluxoid lattices in superconductors; low-temperature ion damage, ion implantation, and ion backscattering in superconductors; inelastic neutron-scattering studies of high-transition-temperature superconductors.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02- (continued)

192. PHYSICAL PROPERTIES OF CERAMICS — $640,000 — 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, C. Wood

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.

193. RESEARCH AND DEVELOPMENT ON PURE MATERIALS — $590,000 — 02-2
L. A. Boatner, M. M. Abraham,
G. C. Battle, W. E. Brundage,
Y. Chen, Y. K. Chang,
T. F. Connolly, C. C. Robinson

Growth and characterization of high-quality single crystals of research materials; preparation of high-purity metals and alloys in rod and foil form; information regarding the physical properties and worldwide availability of research materials provided by the Research Materials Information Center; arc-fusion growth of pure and doped Y_2O_3, MgO, CaO, SrO and other refractory oxides; growth of single crystals of perovskite-structure oxides ($KTaO_3$, $KTa_{1-x}Nb_xO_3$, $K_{1-x}Na_xTaO_3$); electron-beam float-zone growth of refractory metals (Ti, V, Zr, Nb, Ta, W, Ir, Re), alloys and some A-15 compounds (Ti_3Au, Ti_3Pt); float zone growth of high-purity Fe-Cr-Ni alloys, flux growth of tungsten carbide single crystals, preparation and growth of spinel ferrites, special fabrication techniques for thin silicon single crystals; general exploratory crystal growth.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02- (continued)

194. PHOTOPHYSICAL PROCESSES OF SOLAR ENERGY CONVERSION — $455,000 — 02-2
R. F. Wood, M. M. Abraham, B. R. Appleton, J. B. Bates, J. W. Cleland, H. L. Engstrom, B. C. Larson, J. Narayan, T. F. Polgreen, P. P. Pronko, J. C. Wang, R. D. Westbrook, C. W. White, R. T. Young

Initial characterization of single and polycrystalline Si to determine the effects of point defects, defect clusters, dislocation, twin boundaries, stacking faults, grain boundaries, chemical impurities and defect-impurity interactions on electrical and optical properties; thermal neutron transmutation, diffusion, and ion implantation doping experiments for fabrication of p-n or n-p junctions; thermal or laser annealing of lattice damage in reactor irradiated, diffused or ion implanted Si; electrical, optical (including infrared, laser-based infrared and Raman spectroscopy), transmission electron microscopy, x-ray diffuse scattering, electron paramagnetic resonance, surface photovoltage, secondary ion mass spectrometry and Rutherford ion back scattering property measurements; grain boundary compensation in polycrystalline Si by neutron transmutation doping and diffusion; fabrication of test solar cells; study of factors known to degrade solar cell conversion efficiency under single sun and concentrator conditions, junction depth concentration profile and absolute quantum efficiency spectral response measurements.

195. FUNDAMENTAL ASPECTS OF METAL FRACTURE — $220,000 — 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 observation 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.

196. SOLID ELECTROLYTES AND SUPERIONIC CONDUCTIVITY — 02-2
J. B. Bates, T. Kaneda, H. Sato, J. C. Wang

Mechanisms of high ionic conductivity in solid electrolytes such as the beta- and beta''-aluminas and Li_3N; preparation and characterization of new materials based on modification of the beta-alumina structure; techniques include measurements of electrical conductivity and dielectric constant, Raman scattering and infrared absorption, reflection, and emission spectroscopy; experimental results interpreted and correlated by means of model calculations. To be initiated in FY 1979.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02- (continued)

197. THEORY OF CONDENSED MATTER — $760,000 — 02-3
R. F. Wood, J. H. Barrett, J. F. Cooke, H. L. Davis, D. K. Holmes, T. Kaplan, M. E. Mostoller, O. S. Oen, M. Rasolt, M. T. Robinson, M. Ulehla

Electronic structure and optical properties of defects in insulators; superionic conductivity and solid electrolytes; high temperature oxides and carbides; reflection of light atoms from surfaces; near surface diffraction of Auger electrons; interpretation of LEED data; surface studies with back-scattered ions; lattice vibrations in disordered alloys; the coherent potential approximation; vibrational properties around substitutional impurities in insulators; neutron scattering from molecular-like impurities in crystals; band structure calculations in metals and insulators; electronic properties of rare-earth and actinide compounds; electron screening and phonon spectra; lattice dynamics of high T_c superconductors; ferromagnetism in transition metals; spin wave calculations in Ni and Fe; Brillouin zone integration; Heisenberg spin systems; computer simulation of radiation damage and sputtering; radiation damage analysis procedures; correlation of neutron damage with ion bombardment; theory of laser annealing and laser-induced diffusion in semiconductors.

198. LOW-TEMPERATURE RADIATION EFFECTS — $515,000 — 02-4
R. R. Coltman, Jr., C. E. Klabunde, J. K. Redman, J. M. Williams

Fission-neutron damage rates in metals and alloys at 4.7°K; dose-dependent recovery studies of stainless steel and pure and doped V irradiated at 4°K; defect-production studies of alloys and pure and doped metals fast-neutron irradiated near room temperature; normalization of ion and fission-neutron damage in Al 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.

199. X-RAY DIFFRACTION AND ELECTRON MICROSCOPY — $325,000 — 02-4
T. S. Noggle, J. F. Barhorst, B. C. Larson, J. Narayan, S. M. Ohr, J. B. Roberto

Radiation damage resulting from reactor neutrons, 14 MeV neutron and ion irradiations of Au, Cu, Ni, Si, Nb and stainless steel; transmission electron microscopy; x-ray diffuse scattering; single crystal films; laser annealing; defects in MgO; anisotropic elasticity theory of dislocation loops; computer simulation of electron microscopy images; theory of interactions of electrons and x-rays with defects in solids.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02- (continued)

200. ION BOMBARDMENT $260,000 02-4
B. R. Appleton, J. H. Barrett, P. P. Pronko, O. E. Schow III, C. W. White, S. R. Wilson, S. P. Withrow, 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, Cu, Fe, Zn and Al in ion-implanted, laser-annealed Si single crystals; measurements of one-dimensional lattice contraction in B-implanted, laser-annealed Si 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.

201. NORMALIZATION OF ION AND NEUTRON DAMAGE $170,000 02-4
T. S. Noggle, B. R. Appleton, J. Narayan, O. S. Oen, J. M. Williams

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 H, He, Mg, Al, Si, P, S, Cl and Ar ions in Al and Ni ions in Ni; damage theory computations.

202. SURFACE STUDIES AND CATALYSIS $500,000 02-5
L. H. Jenkins, B. R. Appleton, J. H. Barrett, H. L. Davis, J. R. Noonan, M. Rasolt, M. 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 reordered or have interplanar spacings different from those of the bulk; combined techniques of low energy electron diffraction (LEED) and positive ion crystallography of surfaces (PICS) 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.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02- (continued)

203. ION IMPLANTATION — $180,000 — 02-5
B. R. Appleton, P. P. Pronko, O. E. Schow III, N. 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; fabrication of improved efficiency solar cells from boron-implanted laser-annealed silicon; studies of surface alloy formation by laser processing of ion implanted metals; effects of ion implantation on corrosion mechanisms; alteration of superconducting properties by ion implantation doping of superconducting materials; investigations of metastable materials prepared by ion implantation doping and laser processing.

OAK RIDGE NATIONAL LABORATORY
Chemistry Division -03-
O. L. Keller - Phone: (FTS) 850-6444 or 615-483-8611, Ext. 3-6444

204. CHEMICAL STRUCTURE OF ENERGY RELATED MATERIALS — $730,000 — 03-1
W. R. Busing, G. M. Brown, C. K. Johnson, E. Johnson, H. A. Levy, A. H. Narten, W. E. Thiessen

Atomic and molecular arrangements in crystals and in liquids determined by neutron and x-ray diffraction studies; location of light atoms, especially hydrogen; identification of isotopic substituents such as deuterium; development of new computational methods for solving and refining crystal structures; graphic displays for interpreting structure of materials use of intermolecular potentials to compute and extrapolate physical properties. Materials studied include molten salt catalysts for clean fuel synthesis, salt hydrates for thermal energy storage, catalysts for hydrogen production, sterically hindered hydrocarbons, compounds derived from the coal research program, and ionic and organic conductors.

205. MATERIALS CHEMISTRY RELATED TO FUSION REACTOR SYSTEMS — $470,000 — 03-2
J. T. Bell, H. F. Bittner, J. D. Redman, G. M. Begun

High temperature chemical interactions are being defined and characterized in order to determine their advantageous or detrimental effects on materials in energy producing systems. Tritium management in reactor systems will require permeation barriers. Tritium permeation rates through clean metals and alloys and through construction alloys whose surfaces have been oxidized with steam are measured. The chemistry of the steam oxidation of alloys to form effective permeation barriers, and the high temperature chemistry of the oxides are determined. Basic chemical and thermodynamic information is obtained on the tritium fuel cycle; systematic studies are done on the solubilities and on the extraction of hydrogen isotopes in and from breeding blanket materials.

206. PHYSICAL CHEMISTRY OF MOLTEN SALTS IN ENERGY UTILIZATION — $215,000 — 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 used in high temperature battery and fuel cell applications.

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

207. LOCALIZED CORROSION AND STRESS CRACKING PHENOMENA RELATED TO ENERGY TECHNOLOGIES — $325,000 — 03-3
F. A. Posey, A. L. Bacarella, E. J. Kelly, A. A. Palko

Basic electrochemical investigations of mechanisms of corrosion reactions applicable to localized attack of metals (e.g., titanium, stainless steel) needed for understanding corrosion in active and passive states and effects of restrictive geometries (pitting, crevice corrosion, stress corrosion cracking); kinetics of coupled active-passive electrode systems; 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.

208. PREPARATION AND PROPERTIES OF ACTINIDE CARBIDES/NITRIDES — $190,000 — 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, thorium carbides, and plutonium carbides with Cr-Fe-Ni alloys. Thermodynamics properties and compounds in the systems U-C-Cr-Fe-Ni, Th-C-Cr-Fe-Ni, and Pu-Cr-C. Carbothermic conversion of actinide oxides to acinide carbides. 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; ThO_2-ThC_2-C; and *U,Pu)(C,O)-$(U,Pu)C_{1.5}$-C.

209. CHEMICAL ENGINEERING RESEARCH — $190,000 — 03-2
J. S. Watson, S. D. Clinton, R. E. Barker, J. B. Talbot

The measurement and evaluation of materials properties important to chemical processes; the development and evaluation of separation techniques including the study of hydraulic cyclones for removing solid particles from viscous fluids (e.g. coal-derived liquids), and a study of deep-bed filters for removing very small (submicron) particles from organic and aqueous streams.

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

R. Nelson - Phone (FTS) 444-0120 or 509-942-0120

210. METAL-INSULATOR-SEMICONDUCTOR PHOTOVOLTAICS — $80,000 — 01-1
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. Thin film properties--optical transmission, ellipsometry, Auger profile analyses, electron microscopy. Systems of major interest based on single crystal silicon--Au/SiO_2/n-Si and Al/SiO_2/p-Si.

211. SPUTTER-DEPOSITED SOLAR MATERIALS — $150,000 — 01-1
R. Wang, W. T. Pawlewicz,
C. H. Henager, Jr.

Structure-property relationships for thin film photovoltaics, photochemical electrodes and selective photothermal absorbers; electrical, optical and photoelectronic properties of sputter-deposited amorphous Si film; photochemical reactions on semiconductor-electrolyte interface; band-gap, photo-response and electrical properties of sputter-deposited fine-grained and amorphous $SrTiO_3$ and $FeTiO_3$ semiconductors, impurity effects of plasma-sprayed TiO_2 for photoelectrolysis of water; sputter-deposited photothermal absorbers.

212. FUNDAMENTAL STUDIES OF STRESS CORROSION AND CORROSION FATIGUE MECHANISMS — $150,000 — 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 of S, P, Sb and C in Fe and Ni. Relationships between grain boundary chemistry, electrochemical potential and fracture in aqueous solutions. Effect of plastic strain and various gaseous environments on the quantity and distribution of surface segregants will be studied in an Auger electron spectrometer using an in-situ straining stage.

PACIFIC NORTHWEST LABORATORY (continued)

213. OXIDATION, CORROSION AND WEAR RESISTANT FINE-GRAINED MATERIALS — $130,000 — 01-3
M. D. Merz

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, Inconels and Inconel 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: Cu, Ni, $W_{50}Fe_{50}$ and $Fe_{80}B_{20}$; extremely hard alloys and intermetallic components; diskrider method of wear evaluation in vacuum and controlled atmosphere; coefficient of friction.

214. 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; effect of heat treatment under high pressure; 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.

215. RADIATION EFFECTS ON METALS — $400,000 — 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 metals; 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; stress dependence of irradiation creep in nickel; creep of reactor pre-conditioned specimens; modelling of creep behavior; transmission electron microscopy of specimen crept during ion irradiation.

PACIFIC NORTHWEST LABORATORY - (continued)

216. RADIATION DAMAGE IN CERAMICS — $80,000 — 01-4
R. P. Turcotte, W. J. Weber, T. D. Chikalla

Particle induced radiation damage in cubic oxides (fluorite and spinel structures), SiO_2 and complex silicates. Alpha bombardment using actinide sources and preparation of actinide compounds. Structural changes by X-ray diffraction, density, scanning electron microscopy-damage ingrowth and annealing kinetics. Inert gas diffusion/defect interactions in glass.

217. SPUTTERING PARAMETER INFLUENCES ON MATERIAL STRUCTURE AND BEHAVIOR — $150,000 — 01-5
R. Busch, J. W. Pattern, E. D. McClanahan

Effect of sputtering parameters on structure and behavior of deposited materials; columnar growth, types of boundaries, diffusion properties and character of substrate-deposit interface in metallic deposits (Cr, Ni, Co). Effect of deposition rate, substrate temperature and bias, and oxygen partial pressure on stoichiometry and structure of oxide deposits; effect of material parameters, e.g., free energy of formation, cation/anion mass ratio, etc.; oxides of Al, Cr, Ni, and others; study of physical/chemical factors in adherence of oxide deposits to metallic substrates.

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

Examine validity of theory describing scattering of light from metal surfaces by using visible wavelengths and controllably roughed single crystal copper surfaces; optical scattering; etch pits in copper surfaces; chemical crystal polishing; independent sample topography using modified Normarski reflection microscopy; quantitative surface topography analysis; non-contact and non-destructive topography evaluation; fractional wavelength vertical resolution; examine radiation effects on the optical properties of metal reflectors with in-site measurements; copper ion irradiation of single crystal copper reflectors; copper reflectors; laser fusion reflectors; ellipsometry evaluation of optical properties during irradiation.

PACIFIC NORTHWEST LABORATORY - (continued)

219. SPUTTER-DEPOSITED COATINGS FOR OPTICAL APPLICATIONS — $90,000 — 02-2
N. Laegreid, W. T. Pawlewicz, R. Busch, J. S. Hartman

Development of sputter-deposited materials for optical applications; oxides of Ti, Si, Zr, Hf and Ta; fluorides of Mg and Th; SiC, Bn and GaAs; range of refractive indexes; visible or infrared spectral region; property characterization related to stoichiometry and structure, manipulation and control of properties by adjustment of sputtering conditions; refractive index, absorption coefficient and optical band edge by normal incidence transmission/reflection and ellipsometry, X-ray energy spectrometry, X-ray diffraction, scanning electron microscopy and transmission electron microscopy.

220. NANOMETRE MACHINING AND GRINDING DEVELOPMENT - MATERIALS PROPERTIES RESEARCH — $165,000 — 02-5
D. M. Miller, N. Laegreid, R. Busch

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 conves spherical and aspherical surfaces up to one metre diameter. Determine relationship between microstructure and physical/chemical properties of materials and machining/grinding parameters necessary to achieve desired result.

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

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

221. STRESS CORROSION CRACKING — $160,000 — 01-2
W. H. Smyrl

Crack propagation behavior of austenitic and ferritic stainless steels in molten salt environments; low melting mixtures of $AlCl_3$-NaCl-KCl-LiCl, chosen to provide data at same temperature as boiling $MgCl_2$ tests. Determination of hydrogen effects on cracking; measurement of hydrogen permeation and diffusion in the austenitic stainless steels. Electrochemical measurements are conducted in parallel with the stress corrosion tests. New alternating current impedance corrosion techniques have been developed to generate fast, accurate data.

222. ION IMPLANTATION AND DEFECTS IN MATERIALS — $300,000 — 01-3
G. W. Arnold, K. L. Brower,
D. M. Follstaedt, G. B. Krefft,
S. M. Myers, P. S. Peercy,
S. T. Picraux, F. L. Vook

Ion beam modification and analysis of near surface regions of solids. Laser annealing of implanted and amorphous solids, H concentration measurements and bonding observations in crystalline and amorphous Si, EPR and optical investigation of radiation-induced defects and H in SiO_2 glasses, surface recrystallization of glasses and fused SiO_2. Ion implantation metallurgy: formation of equilibrium and nonequilibrium alloys, 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.

223. EROSION AND WEAR IN A FLUID ENVIRONMENT — $100,000 — 01-5
R. E. Cuthrell, H. O. Pierson,
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 conditions, as determined using acoustic emission 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)

224. SURFACE PHYSICS RESEARCH — $200,000 — 02-2
J. E. Houston, J. A. Panitz
R. R. Rye, P. J. Feibelman,
D. R. Jennison, F. L. Vook

Field-desorption microscopic imaging of the structures of molecules adsorbed on metal surfaces. Mass and site specific, two-dimensional images are recorded with Angstrom spatial resolution. Auger electron spectroscopy has been demonstrated both experimentally and theoretically to be a unique probe of local chemical environment using the correlated spectral results from selected series of gas-phase molecules.

225. DEVELOPMENT OF FIELD-DESORPTION MICROSCOPE FOR BIOMOLECULE IMAGING — 02-5
J. A. Panitz, J. E. Houston,
F. L. Vook

An instrument is being developed utilizing field-desorption and TEM techniques to obtain structural images of biological molecules with approximately 1 Å resolution. This apparatus will include the capabilities of time-of-flight mass analysis on desorbed species and surface sample dosing without breaking vacuum. To start in FY 1979.

226. HYDROGEN PRODUCTION BY SOLAR PHOTO-ASSISTED ELECTROLYTIC DECOMPOSITION OF WATER — $130,000 — 02-2
M. A. Butler, D. S. Ginley,
M. L. Knotek, B. Morosin,
J. E. Schirber

Investigation of the feasibility of H production by photoassisted electrolysis of H_2O at chemically inert semiconductor electrodes. Electrochemical behavior of aqueous and related systems including electrospectroscopy of reaction intermediates; variation of semiconductor electrode material properties, including surface film passivation as well as activation. Surface studies on a microscopic basis to understand basic reaction steps; theoretical studies to model the behavior of material property characteristics of electrodes.

SANDIA LABORATORIES (continued)

227. STUDIES OF THE VAPOR PHASE OF THE CHEMICAL-VAPOR-DEPOSITION PROCESS — $60,000 — 02-5
G. H. Miller, A. W. Johnson, A. J. Mulac, P. J. Hargis

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

SANDIA LABORATORIES
Livermore, California 94550

228. GASES IN METALS $220,000 01-2
W. D. Wilson, G. J. Thomas,
W. A. Swansiger, M. I. Baskes,
J. H. Holbrook, 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.

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 — $ 67,846 — 02-2
J. M. Cowley - Dept. of Physics
Phone: (602)-965-6459

New techniques for the study of the surface structure of crystalline solids by diffraction and imaging with electrons have been evolved. A new type of instrument has been built using an ultra-high vacuum system and allowing a combination of medium energy (1-10 keV), electron diffraction and scanning electron microscopy with a novel procedure for forming images by the use of diffracted beams. Near atomic resolution is being achieved on surface imaging by transmission.

UNIVERSITY OF ARIZONA

302. STUDY OF GAS EVOLUTION THRESHOLDS AT SEMICONDUCTOR-ELECTROLYTE INTERFACES USING DIFFERENTIAL REFLECTANCE SPECTROSCOPY — $ 72,720 — 02-2
S. Sari - Optical Sciences Center
Phone: (602)-884-3025

This study examines a number of aspects of gas evolution, properties of adsorbed layers and reaction processes at semi-conductor-electrolyte interfaces. Optical spectroscopic methods utilizing sensitive differential reflectance techniques will be emphasized. Electronic and molecular processes at solid-liquid interfaces, in particular the metal-liquid boundary under electrolytic action, will be studied.

BROWN UNIVERSITY

303. A COMBINED MACROSCOPIC AND MICROSCOPIC APPROACH TO THE FRACTURE OF METALS — $121,000 — 01-2
J. Gurland - Division of Engineering
Phone: (401)-863-2628
J. R. Rice - Division of Engineering
Phone: (401)-863-2866

Evaluation of deformation and fracture of metal alloys -- primarily steels; plasticity considerations in ductile crack growth; relation of microscale fracture mechanisms to macroscopic fracture mechanics; shear localization; embrittlement due to hydrogen or grain boundary segregation.

CALIFORNIA INSTITUTE OF TECHNOLOGY

304. STUDIES OF ALLOY STRUCTURES AND PROPERTIES — $140,000 — 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.

305. A STUDY OF METAL HYDRIDES AND IONIC CONDUCTORS WITH NUCLEAR MAGNETIC RESONANCE TECHNIQUES — $ 70,000 — 03-1
R. W. Vaughan - Chemistry and Chemical Engineering Dept.
Phone: (213)-795-6811, X1183

Multiple pulsed nuclear magnetic techniques to investigate chemical and electronic bonding in binary metal hydrides. Materials to be studied include the alkaline-earth hydrides and a group of "cluster" covalent hydrides of Ru and Os containing covalently linked CO. Additional systems to be studied will include polycrystalline β- and β"-alumina, alkali-doped βPbF_2 and CdF_2. A widely-based effort will be made to employ NMR techniques in the study of ionic mobility.

306. THE PRESSURE DEPENDENCE OF THE MECHANICAL PROPERTIES OF POLYMERS — $ 96,000 — 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/LOS ANGELES

307. IRRADIATION INDUCED PRECIPITATION IN PALLADIUM-BASE ALLOYS — $ 75,000 — 01-4

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

Experimental study of irradiation-induced precipitation in binary Pd-base alloys; 400 to 1000°C; proton, electron, and heavy-ion irradiations; TEM and auger spectroscopy; alloys of Pd with V, Cr, Mn, Fe, Zn, Cd, Nb, Mo, Ta, W, Ag, Ni, and Cu; effect of solute-solvent atomic-size misfit; effect of dose rate; stability of the precipitate; relationship between irradiation-induced precipitate and void swelling.

308. SEMICONDUCTOR EUTECTICS FOR ENERGY CONVERSION — $ 64,240 — 02-2

A. S. Yue - Materials Department
Phone: (213)-825-4166

This research involves the preparation of SnSe (p-type) and $SnSe_2$ (n-type) compounds and a lamellar SnSe-$SnSe_2$ eutectic, and the investigation of semiconductor behavior of these compounds and the eutectic. Because of the extremely high p-n junction density of the SnSe-$SnSe_2$ eutectic, it will be an ideal material for efficient conversion of solar energy into electricity. Liquid phase epitaxy will also be attempted. In addition the GaAs-Ge eutectic system will be studied.

UNIVERSITY OF CALIFORNIA/RIVERSIDE

309. THEORETICAL ASPECTS OF SUPERCONDUCTOR BEHAVIOR — $ 48,127 — 02-3

E. Simanek - Physics Department
Phone: (714)-787-5640

Theoretical study of the properties of inhomogeneous superconducting films and aggregates of ultrafine metallic particles; temperature dependence of the order parameter to be calculated from the model of random superconductivity to interpret tunneling studies of Al films; effects of Josephson coupling between particles in aggregates.

UNIVERSITY OF CALIFORNIA/SAN DIEGO

310. THE RESPONSE OF SUPERCONDUCTORS TO VARIATIONS IN IMPURITY CONTENT AND APPLIED PRESSURE — $154,356 — 02-2

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

This is an experimental research program to investigate the response of superconductivity to variations in impurity content, throughout the entire range of solute magnetic character, and applied pressure. 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.

311. RESEARCH ON THERMOPHYSICAL PROPERTIES OF MATERIALS — $225,393 — 02-2

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

The orbital properties of superfluid ^3He-A are some of the most novel of this superfluid. Using ultrasonic attenuation as a probe both A and B phases of liquid ^3He will be investigated. In addition to this low temperature work, a new effort on liquid engines will be inaugurated.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA

312. RESONANCE STUDIES OF SUPERIONIC CONDUCTORS — $ 58,995 — 02-2

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

NMR and EPR study of superionic and related compounds; study of phase transition in PbF_2 at 310°C; use of EPR to study electrode-electrolyte interfaces; F^{19} NMR in KMn_xMg_{1-x} and in Mn-doped PbF_3; EPR of ion interchange in rutile structure crystals.

CARNEGIE-MELLON UNIVERSITY

313. 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

Analysis of the internal centrifugal zone growth (ICZG) crystal growing process for refractory materials and composites; theoretical modeling and experimental research to confirm model predictions; modeling of solid-liquid interfacial energies; chemical potentials of stressed solids; morphological stability of ceramics.

CASE WESTERN RESERVE UNIVERSITY

314. STUDY OF COUPLED DIFFUSION PHENOMENA IN MULTICOMPONENT GLASSES AND GLASS FORMING LIQUIDS — $ 97,650 — 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.

315. PLASTIC DEFORMATION IN OXIDE CERAMICS — $ 66,500 — 01-2
A. H. Heuer - Dept. of Metallurgical and Materials Sciences
Phone: (216)-368-4224

Transmission electron microscopy of dislocation structures and interactions during high temperature deformation of single crystal oxides; effects of stoichiometry; interactions between vacancies, interstitials, clusters and moving dislocations; loop annihilation kinetics and diffusion coefficients.

316. EXPERIMENTS IN HIGH VOLTAGE ELECTRON MICROSCOPY — $100,087 — 01-4
T. E. Mitchell and L. W. Hobbs - Dept. of Metallurgy and Materials Science
Phone: (216)-368-4210

High voltage electron microscopy of in-situ radiation damage and kinetic process enhancement; threshold displacement determinations in metals and ceramics; radiation effects in metallic alloys with particular reference to the role of defects; radiation defect stabilization in ceramics; defect aggregation, loop growth kinetics, vacancy condensation and void formation, swelling, and radiation-induced phase decomposition in ceramics.

317. ELASTIC AND PLASTIC STRAINS AND THE STRESS CORROSION CRACKING OF AUSTENITIC STAINLESS STEELS — $ 46,000 — 01-2
A. R. Troiano - Dept. of Metallurgy and Materials Science
Phone: (216)-368-4234

Stress corrosion cracking in austenitic stainless steels in aqueous chloride solutions; electrochemical potentials of steels with various martensite contents and after cold rolling; passive film structure and stability.

CASE WESTERN RESERVE UNIVERSITY (Continued)

318. ENVIRONMENTAL REACTIONS AND THEIR EFFECTS ON MECHANICAL BEHAVIOR OF METALLIC MATERIALS — $ 60,000 — 01-2
R. Gibala - Department of Metallurgy and Materials Science
Phone: (216)-368-4210

Interactions among bulk and near-surface defect structures in metals and influence on mechanical behavior; softening of Nb and Ta coated with oxide below 77°K; stress differential effect; dislocation nucleation in stress gradients; effect of O on deformation in Nb-H alloys and hydride coherency; H embrittlement of low alloy steels; techniques used -- HVEM and TEM, electrical resistivity, mechanical testing.

CATHOLIC UNIVERSITY OF AMERICA

319. IONIC TRANSPORT AND ELECTRICAL RELAXATION IN GLASS — $ 47,800 — 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 CHICAGO

320. THE STUDY OF PHONONS AND ELECTRONIC PROCESSES IN ORDERED AND DISORDERED SOLIDS — $ 64,929 — 02-2
S. A. Solin - Dept. of Physics
Phone: (312)-753-8224

Raman, infrared and x-ray techniques used to investigate disordered, partially ordered and ordered solids. Specifically, amorphous diamond films, chalcogenide glasses and alloys, graphite intercalates, sodium tungsten bronzes, graphite and tungsten trioxide are being studied.

UNIVERSITY OF CINCINNATI

321. FLUX PINNING AND FLUX FLOW STUDIES IN SUPERCONDUCTORS USING FLUX FLOW NOISE TECHNIQUES — $ 51,508 — 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.

CLARKSON COLLEGE OF TECHNOLOGY

322. CONDENSATION PROCESSES IN COAL COMBUSTION PRODUCTS — $ 39,000 — 03-3

J. L. Katz - Dept. of Chemical Engineering
Phone: (315)-268-6652
M. C. Donohue - Dept. of Chemical Engineering
Phone: (315)-268-6663

Theoretical and experimental study of complex condensation processes occurring in coal-fired energy systems; study of materials problems arising from condensation of slag.

COLORADO ENERGY RESEARCH INSTITUTE
(COLORADO SCHOOL OF MINES AND COLORADO STATE UNIVERSITY)

323. HYDROGEN AND METHANE SYNTHESES THROUGH RADIATION CATALYSIS — $161,990 — 02-2

J. G. Morse, Colorado School of Mines
Phone: (303)-279-0300
J. DuBow, Colorado State University
Phone: (303)-491-8235

Ionizing radiation has been shown to increase reaction rates by up to two orders of magnitude. The radiation generates electron-hole pairs through optical or radioactive stimulus and subsequent excitation via sub-damage threshold radiation enables the continuous generation of metastable high energy carrier pairs. This research is involved with a study of radiation-induced catalysis examining mechanisms of energy transfer from the catalyst to its adsorbed reactant in an ionizing radiation environment.

COLORADO SCHOOL OF MINES

324. FERROUS ALLOY METALLURGY - LIQUID LITHIUM CORROSION AND WELDING — $ 97,000 — 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; 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.

UNIVERSITY OF COLORADO

325. CRITICAL SCATTERING OF LASER LIGHT BY BULK FLUIDS AND THIN — $107,385 — 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

326. DEFECT INTERACTIONS AT HIGH CONCENTRATIONS IN SOLID-OXIDE ELECTROLYTES — $ 43,291 — 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.

COLUMBIA UNIVERSITY (Continued)

327. HIGH TEMPERATURE PROPERTIES OF NUCLEAR REACTOR COOLANTS AND THERMODYNAMIC POWER CYCLE WORKING FLUIDS — $ 47,594 — 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

328. ELECTRON-DISLOCATION INTERACTIONS AT LOW TEMPERATURES — $51,218 — 01-2
J. M. Galligan - Dept. of Metallurgy
Phone: (203)-486-3541

Electron and phonon drag on dislocations; use of superconductor-normal transition to alter electronic state; dislocation-fluxoid interactions; flow stress-field interactions in normal metals; dislocation-interstitial interactions; orientation effects; Pb, Pb-Sn, Pb-Ag, Cu, and Zn.

329. CLUSTER CARBURIZING — $ 32,500 — 01-1
J. E. Morral - Dept. of Metallurgy and Inst. of Materials Sciences
Phone: (203)-486-2923

Carburization of Ta-Hf and Nb-Hf alloys on pre-existing solute clusters or on dislocation network; theory of subscale formation; NbC-HfC phase diagram.

330. ELECTRODE POLARIZATION STUDIES IN HOT CORROSION SYSTEMS — $ 42,200 — 01-1
O. F. Devereux - Dept. of Metallurgy
Phone: (203)-486-4714

Elevated temperature corrosion of metals -- Fe, Ni, Cr and their alloys -- in gases and liquids with high S contents; thermodynamic modelling of activities in multicomponent systems; measurement of electrochemical behavior of Fe and Ni in molten Na_2CO_3; development of Al_2O_3 reference electrode.

CORNELL UNIVERSITY

331. MECHANICAL PROPERTIES OF CRYSTALLINE SOLIDS — $ 87,021 — 01-2

Che-Yu Li - Dept. of Materials Science and Engineering
Phone: (607)-256-4349
E. W. Hart - Dept. of Materials Science and Engineering
Phone: (607)-256-4853

Development of concepts and methods for characterizing mechanical properties of solids based on the state variable approach; load relaxation of metallic glasses; load relaxation of Zircaloy-4; growth kinetics of grain boundary methane bubbles in Ni; creep damage in the form of grain boundary cavities in Zircaloy-4; non-elastic deformation and recovery in Al and Ni.

332. DEFECTS IN METAL CRYSTALS — $211,948 — 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; transmission sputtering of gold thin films by low energy zenon ions; range of focussed collision replacement sequences; recovery behavior of proton irradiated tungsten; mobility and range of implanted low energy helium in tungsten.

333. MECHANICAL BEHAVIOR OF MATERIALS AND STRUCTURAL ELEMENTS AT ELEVATED TEMPERATURES — $ 75,000 — 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)-256-4853

Analytical and experimental research on constitutive equation for mechanical deformation; deformation of thick walled spheres and cylinders for all symmetrical loading methods; computer programs for the predicted deformation for a variety of loading conditions for spherical and cylindrical geometry; testing and comparison for beams under long and short time test conditions and under many loading sequences.

CORNELL UNIVERSITY (Continued)

334. INFLUENCE OF GRAIN BOUNDARIES ON THE ELECTRICAL TRANSPORT PROPERTIES OF POLYCRYSTALLINE SI FILMS — $ 52,600 — 01-1
D. G. Ast - Dept. of Materials Science and Engineering
Phone: (607)-256-4140

Evaluation of structure and electrical activity of defects in crystalline Si; tilt and twist boundaries in hot-pressed Si; twin boundaries in Si produced by edge-defined film-fed growth; techniques used: TEM, SEM, EBIC in SEM.

335. PROBABILISTIC MODELS OF THE STRESS-RUPTURE OF COMPOSITE MATERIALS — $ 53,000 — 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 considerations; weakest link rule scaling of composite size effect.

336. ENVIRONMENT AND FRACTURE — $ 66,000 — 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.

337. HIGH TEMPERATURE MECHANICAL BEHAVIOR OF SILICON NITRIDE — $ 56,824 — 01-2
R. Raj - Dept. of Materials Science and Engineering
Phone: (607)-256-4040

Crack initiation and crack growth leading to failure in silicon nitride ceramics at elevated temperatures; relation of microstructure to deformation and fracture; effects of grain size, porosity, composition, volume fraction and distribution of intergranular phases; grain boundaries; slow crack growth; internal friction, transmission electron microscopy.

CORNELL UNIVERSITY (Continued)

338. INELASTIC DEFORMATION IN NON-METALLIC CRYSTALLINE SOLIDS — $ 48,600 — 01-2

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

Plastic deformation of germanium and transition metal carbides; load relaxation and constant strain rate experiments; transmission electron microscopy; dislocation etch pit studies on germanium; effects of charged impurities on dislocation dynamics in germanium; correlation of dislocation substructures to a mechanical equation of state.

DARTMOUTH COLLEGE

339. THEORY OF ELECTRON-PHONON SCATTERING EFFECTS IN METALS — $ 32,960 — 02-3

W. E. Lawrence - Dept. of Physics and Astronomy
Phone: (603)-646-2963

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

340. EXPERIMENTAL DETERMINATION OF THE TEMPERATURE DEPENDENCE OF METALLIC WORK FUNCTIONS AT LOW TEMPERATURES — $ 30,809 — 02-2

P. B. Pipes - Dept. of Physics and Astronomy
Phone: (603)-646-2962

The effect of the superconducting transition on the temperature dependence of the contact potential in niobium will be studied as a function of magnetic field and surface preparation to determine the relative importance of bulk and surface effects. The influence of adsorbed ^4He will also be studied.

DREXEL UNIVERSITY

341. STRAIN HARDENING AND DUCTILITY OF IRON: AXISYMMETRIC VS. PLANE STRAIN ELONGATION — $ 40,900 — 01-2

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

Correlation of strain hardening of iron and steel with dislocation structure developed during secondary fabrication; axisymmetric and plane strain deformation; technique used; high voltage electron microscopy, wire and strip drawing, tensile testing.

UNIVERSITY OF FLORIDA

342. SYNTHESIS AND CHARACTERIZATION OF NOVEL POLYMERS FROM NON-PETROLEUM SOURCES — $ 70,000 — 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.

343. DEFORMATION PROCESSES IN REFRACTORY METALS — $ 44,000 — 01-2

R. E. Reed-Hill - Dept. of Materials Science and Engineering
Phone: (904)-392-1456

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

344. QUANTITATIVE ANALYSIS OF SOLUTE SEGREGATION IN ALLOYS BY TRANSMISSION ELECTRON MICROSCOPY — $ 53,800 — 01-1

J. J. Hren - Dept. of Metallurical and Materials Engineering
Phone: (904)-392-1462
C. S. Hartley - Dept. of Metallurgical and Materials Engineering
Phone: (904)-392-1457

Experimental and analytical study of defect images in TEM; effects of local strain fields and elastic anisotropy; catalogue of simulated dislocation images for face-centered-cubic and body centered-cubic-metals; techniques used: computer simulation, HVEM.

GEORGIA INSTITUTE OF TECHNOLOGY

346. THE STRUCTURE AND REACTIVITY OF HETEROGENEOUS SURFACES AND STUDIES OF THE GEOMETRY OF SURFACE COMPLEXES — $ 84,025

U. Landman - Dept. of Physics
Phone: (404)-894-3368
E. W. Montroll - Dept. of Physics & Astronomy
Phone: (716)-275-4371

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.

347. INVESTIGATIONS OF RELATIONSHIPS BETWEEN MICROSTRUCTURE, MAGNETIC PROPERTIES AND THE HYDRIDING PROCESSES IN INTERMETALLIC COMPOUNDS OF RARE EARTH AND TRANSITION METALS — $ 82,000 — 01-1

B. R. Livesay - Applied Sciences Laboratory
Phone: (404)-894-3489

Studies of both thin and thick films of FeTi and certain RT_5 alloy systems where R represents a rare earth and T a transition metal element; microstructure, magnetic properties, electronic structure, and pressure-composition relationships caused by modifications to the alloy system; surface coatings, ternary alloy additions and thermal mechanical effects; TEM, AES and SEM; hydride nucleation sites, growth mechanisms, hydride decomposition and hysteresis and stability.

UNIVERSITY OF HAWAII

347. PRESSURE DERIVATIVES OF ELASTIC MODULI IN B.C.C. TRANSITION METALS AND THEIR SOLID SOLUTIONS — $ 48,747 — 02-2

M. H. Manghnani - Dept. of Geology and Geophysics
Phone: (808)-948-8111

Investigation of the pressure dependence of the structure and elastic properties of bcc solid solutions alloys of the transition elements of groups IV B, V B, and VI B using ultrasonic interferometry to 5 Kbar, and x-ray diffraction techniques up to 200 kbar. The relationship between the electronic band structure and the elastic properties of these materials will be studied.

UNIVERSITY OF HOUSTON

349. MICROSTRUCTURAL STUDIES OF HYDROGEN AND OTHER INTERSTITIAL DEFECTS IN BCC REFRACTORY METALS — $ 65,800 — 02-2
S. C. Moss - Dept. of Physics
Phone: (713)-749-2840

X-ray and neutron diffraction study of H and D occupancy in V, Ta, Nb; symmetry of interstitial-induced strain field; short-range and long-range order; positron annihilation in Ta-H alloys related to Fermi surface modifications.

ILLINOIS INSTITUTE OF TECHNOLOGY

350. DIFFUSION MECHANISMS AND DEGRADATION OF ENVIRONMENTALLY SENSITIVE COMPOSITE MATERIALS — $ 48,400 — 01-2
L. J. Broutman - Dept. of Metallurgy and Materials Engineering
Phone: (312)-567-3049

Investigation of moisture diffusion mechanisms and environmental degradation in graphite fiber reinforced epoxy composites; comparison with matrix behavior alone; influence of stress on permeation and fiber-matrix decohesion.

351. ELECTROCHEMISTRY OF ACETYLIDES, NITRIDES AND CARBON CATHODES IN MOLTEN HALIDES — $ 42,000 — 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.

LEHIGH UNIVERSITY

352. PRESSURE SINTERING AND CREEP DEFORMATION - A JOINT MODELLING APPROACH — $ 48,707 — 01-1

M. Notis - Dept. of Metallurgy and Materials Sciences
Phone: (215)-691-7000, X636

Correlation of the kinetics of later stages of densification by pressure sintering with creep deformation; determination of rate-controlling mechanisms; effects of stress, temperature, microstructure, stoichiometry, and impurity content; quantitative relationships via deformation maps; transmission electron microscopy of dislocation substructures; grain boundary segregation; grain boundary deformation; CoO, NiO, and $MgAl_2O_4$.

UNIVERSITY OF MARYLAND

353. ALLOY STRENGTHENING DUE TO ATOMIC ORDER — $ 53,600 — 01-2

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

Mathematical modelling of cracks and interfaces in metals in terms of dislocation arrays; differential geometry description of elastic and plastic distortions and tearing; cyclic stress and tensile vs shear crack considerations; development of scaling methods.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

354. MICROMECHANICAL MODELLING OF MICRO-STRUCTURAL DAMAGE AT ELEVATED TEMPERATURE DURING CREEP OF SUPERALLOYS FOR ENERGY APPLICATIONS — $122,700 — 01-2

A. S. Argon - Dept. of Mechanical Engineering
Phone: (617)-253-2217
F. A. McClintock - Dept. of Mechanical Engineering
Phone: (617)-243-2217

Investigation of crack nucleation and growth during creep of metal alloys; analytical description of singularities such as particle-matrix decohesion at grain boundaries; modelling boundary sliding and crack initiation and growth; materials --- stainless steel, ckel alloys.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (Continued)

355. KINETIC PROCESSES AT GRAIN BOUNDARIES — $ 94,000 — 01-1

R. W. Balluffi - Dept. of Materials Science and Engineering
Phone: (607)-256-4135

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.

356. HIGH TEMPERATURE PROPERTIES AND PROCESSES IN CERAMICS — $124,000 — 01-3

H. K. Bowen - Dept. of Ceramics
Phone: (617)-253-6892
B. J. Wuensch - Dept. of Ceramics
Phone: (617)-253-6889

Effects of large temperature gradients on atomic transport behavior in ceramics; theory of time dependent thermomigration; kinetic and thermodynamic effects in transport theory; ion microprobe analysis; oxygen tracer diffusion; Seebeck effect; pore migration; FeO, $FeAl_2O_4$-Fe_3O_4 solid solutions, KCl, NaCl, Al_2O_3.

357. PROCESSING STUDIES OF POWDER METALLURGICALLY PRODUCED HIGH TEMPERATURE ALLOYS — $ 46,800 — 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.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (Continued)

358. BASIC RESEARCH IN C TALLINE AND NONCRYSTALLINE MIC SYSTEMS — $585,000 — 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 gr n boundary segregation in MgO.

359. LOW TEMPERATURE AND NEUTRON PHYSICS STUDIES — $166,322 — 02-1
C. G. Shull - Dept. of Physics
Phone: (617)-253-4521

The neutron spectrometers currently being modernized at the reconstructed MIT Research Reactor have been reinstalled and used for studies in materials characterization and fundamental neutron physics. The high flux reactor at ORNL will also be used. These studies will include further work on the diamagnetization structure of bismuth, de Haas-van Alphen scattering effects and on neutron interferometry development and uses.

360. ELECTRONIC CONDUCTION IN SOLID OXIDE ELECTROLYTES — $ 60,000 — 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 nductivity thermoelectric power, and ionic transference number. rostructural studies of second phases, grain boundary effects segregation.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (Continued)

361. SPECTROSCOPIC INVESTIGATIONS OF SMALL MOLECULE INTERACTIONS ON METAL OXIDE SURFACES — $ 54,000 — 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. A BASIC STUDY OF ELECTROSLAG WELDING — $ 60,000 — 01-5

J. Szekely - Dept. of Materials Science and Engineering
Phone: (617)-253-6885
T. Eagar - Dept. of Materials Science and Engineering
Phone: (617)-253-3236

Study of electroslag welding of low alloy steels; two dimensional analysis of heat and fluid flows for orthogonal and radial weld geometries; evaluation of weldment macro- and microstructure and hardness profiles.

MICHIGAN TECHNOLOGICAL UNIVERSITY

363. 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 Metallurigal Engineering
Phone: (906)-487-2630

Grain boundary segregation in metals and effect on properties; stress corrosion cracking, theory and experiment; Auger photoelectron 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 Cu by Pb.

UNIVERSITY OF MINNESOTA

364. EXPERIMENTAL INVESTIGATIONS IN SOLID STATE AND LOW TEMPERATURE PHYSICS — $190,000 — 02-2

A. M. Goldman - Dept. of Physics
Phone: (612)-373-5480
W. V. Weyhmann - Dept. of Physics
Phone: (612)-373-5481
W. Zimmermann, Jr. - Dept. of Physics
Phone: (612)-373-9787

Measurements of pair-field susceptibility will be done as well as fluctuation phenomena, and the interaction of long-range magnetic order and superconductivity. The metal-nonmetal transition in Hg_xSe_{1-x} will be completed. The magnetic studies will be carried out at temperatures in the 1-100 mK range, and applied fields of 10 G to 80 KG will be used to study the static and dynamic properties of weak magnetic materials in the critical region. Paramagnetic materials for magnetic refrigerators above 1 K will be investigated in a series of promising compounds.

NEW MEXICO INSTITUTE OF MINING AND TECHNOLOGY

365. MICROSTRUCTURE AND MECHANICAL PROPERTIES OF COATINGS FOR SOLAR COLLECTORS — $ 65,000 — 01-1

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

CITY UNIVERSITY OF NEW YORK

366. NONADIABATIC APPROACH TO VIBRONICALLY ASSISTED RADIATION AND RADIATIONLESS TRANSITIONS — $ 56,774 — 02-3
M. Lax - Dept. of Physics
Phone: (212)-690-6864

A relation will be developed between the vibronically assisted radiative cross-section and that for radiationless transitions. Calculations will be made of the cross section associated with a true multiphonon process. The method proposed will treat the nuclei classically but avoid the adiabatic approximation and will be patterned after a method due to Landau and Zener. A specific calculation is the rate of piezoelectric and deformation potential production of acoustic phonons during nonradiative capture in GaAs.

STATE UNIVERSITY OF NEW YORK/BINGHAMTON

367. ENERGIES AND BONDING IN MANGANESE PHOSPHIDES — $ 22,000 — 03-3
C. E. Myers - Dept. of Chemistry
Phone: (607)-798-2269

Systematic interrelations among the atomization enthalpies, electron binding energies, bond energies in manganese phosphides in relationship with other transition metal phosphides. Dissociation pressure measurements of two-phase regions in the Mn-P system, as well as X-ray photoelectron spectra of manganese phosphides in comparison with phosphides of iron.

STATE UNIVERSITY OF NEW YORK/STONY BROOK

368. PREPARATION, CHARACTERIZATION AND USE OF METAL HYDRIDES FOR FUEL SYSTEMS — $ 49,000 — 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; photodecomposition 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.

STATE UNIVERSITY OF NEW YORK/STONY BROOK (Continued)

369. 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.

UNIVERSITY OF NORTH CAROLINA

370. THE STRUCTURE OF NEUTRON DAMAGE IN IONIC REFRACTORY OXIDES — $ 51,915

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

Structure of neutron damage in ionic refractory oxides; lattice expansion, lattice defects, and associated charge states; optical absorption; luminescent emission; electron spin resonance; dimensional charge measurements; elastic constant measurements; MgO, Al_2O_3, $MgAl_2O_4$, $Y_3Al_5O_{12}$, and TiO_2.

NORTHEASTERN UNIVERSITY

371. EQUILIBRIUM AND TRANSPORT PROPERTIES OF DISORDERED TRANSITION AND NOBLE METAL ALLOYS — $ 37,639

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 approximation (ATA) applied to a variety of disordered alloys with noble metal base and polyvalent solute.

NORTHEASTERN UNIVERSITY (Continued)

372. STUDIES OF DISLOCATION MOTION AND SLIDING FRICTION — $ 47,124 — 02-3

J. Sokoloff - Dept. of Physics
Phone: (617)-437-2931

The Frenkel-Kontorova model will be used to study the epitaxial growth of films and how they get pinned in place even when its periodicity is not commensurate with the substrate. In addition the damping of dislocation motion and friction between sliding crystal planes will be studied in a modified Frenkel-Kontorova model in which phonons are created. The method will also be applied to a model of superionic conduction.

NORTHWESTERN UNIVERSITY

373. INVESTIGATION OF DISPERSED IRON ALLOY CATALYSTS IN THE CARBON MONOXIDE-HYDROGEN SYNTHESIS REACTION — $ 78,000 — 01-3

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

Study of highly dispersed bimetallic 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 caribde structure using temperature variation in Mossbauer experimental experiments to characterize the magnetic saturation structure. Measurement of local temperature rise on the carbide as a consequence of the synthesis reaction.

374. STUDIES OF METAL-SEMICONDUCTOR INTERFACES IN CATALYSIS AND ENERGY CONVERSION — $ 60,000 — 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)

375. EFFECT OF POINT DEFECTS ON MECHANICAL PROPERTIES OF METALS — $ 58,400 — 01-4
M. Meshii - Dept. of Materials Science
Phone: (312)-492-3213

Deformation of metals at low temperature, surface film softening of Ni-coated Fe; electron irradiation of Nb sheet, effects of crystallographic orientation, temperature, strain rate and prestrain on strength, dislocation motion, and slip band formation.

376. BASIC RESEARCH ON CERAMIC MATERIALS FOR ENERGY STORAGE AND CONVERSION SYSTEMS — $ 65,000 — 01-1
D. H. Whitmore - Dept. of Materials Science
Phone: (312)-492-3533

Experimental determination of the factors affecting charge and mass transport in solid electrolyte and electrode materials; single crystal growth; electrical conductivity, tracer diffusion, nuclear magnetic resonance, dielectric loss, ionic thermal currents, and laser Raman spectroscopy; study of electrolyte polarization by complex admittance analysis in sodium doped β" alumina; solid solution electrodes for lithium and sodium cells; growth of single crystal zirconium sulfide; zirconium selenide; layered compounds; fast ion conductors; various antimonates; mixed chlorides; lithium titanates, indium and thallium ternary iodides.

UNIVERSITY OF NOTRE DAME

377. PORE SHRINKAGE AND OSTWALD RIPENING IN METALLIC SYSTEMS — $ 54,000 — 01-1
G. C. Kuczynski - Dept. of Metallurgy Engineering and Materials Science
Phone: (219)-283-6151
C. W. Allen - Dept. of Metallurgy Engineering and Materials Science
Phone: (219)-283-7456

Experimental study of the kinetics of pore shrinkage in porous structures; theoretical and experimental investigation of Ostwald ripening of pores, second phases, and supported catalysts; in-situ transmission electron microscopy; Ni-Al and Au-Fe alloys.

OHIO STATE UNIVERSITY

378. FUNDAMENTAL STUDIES OF METAL FLUORINATION REACTIONS — $ 65,800 — 01-3
R. Rapp - Dept. of Metallurgical Engineering
Phone: (614)-422-6178

Study of structural, thermodynamic, and transport properties pertinent to solid state electrolytes and fluorination of Cu and Ni; electrical conductivity, defect structures and transport mechanisms in CaF_2, NiF_3, and PbF_2.

379. HYDROGEN ATTACK OF STEEL — $ 41,257 — 01-2
P. G. Shewmon - Dept. of Metallurgical Engineering
Phone: (614)-422-2491

Experimental investigation of the microscopic processes that limit the nucleation and growth of methane bubbles during hydrogen attack of steel; effects of deoxidation practice, microstructure, and inclusions; mechanism and kinetics of hydrogen attack; metallography of fracture kinetics and volume-change kinetics.

380. CORROSION, STRESS CORROSION CRACKING AND ELECTROCHEMISTRY OF THE IRON AND NICKEL BASE ALLOYS IN CAUSTIC ENVIRONMENTS — $ 61,400 — 01-1
R. W. Staehle - Dept. of Metallurgical Engineering
Phone: (614)-422-6255
A. K. Agrawal - Dept. of Metallurgical Engineering
Phone: (614)-422-1634

Corrosion of Fe, Ni, and Cu and their alloys in caustic and sulfide aqueous environments between ambient and 150°C; surface film formation and rupture and correlation with alloy composition in SCC of austenitic stainless steels; effectiveness of inhibitors, including chromate union, related to redox couples; techniques used: slow and fast straining electrode, potentiodynamic scans, controlled potential coulometry.

OKLAHOMA STATE UNIVERSITY

381. 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

382. CERAMIC RESEARCH — $ 40,000 — 01-2
R. C. Bradt - Dept. of Materials Science
Phone: (814)-865-4700, X4631
J. H. Hoke - Dept. of Materials Science
Phone: (814)-865-4700, X2071

Transformational and isothermal superplasticity in two phase eutectoid systems such as Bi_2O_3 - Sm_2O_3 and in single phase Bi_2 WO_6-type compounds; effects of stoichiometry on fracture and elastic properties of TiO_{2-x}, FeO_{1+x} and $MgAl_2O_4$ spinel; K_{Ic} measurements; subcritical crack growth; fracture.

383. GRAIN BOUNDARY DIFFUSION AND GRAIN BOUNDARY CHEMISTRY OF CR-DOPED MAGNESIUM OXIDE — $ 18,500 — 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.

384. STUDIES OF MECHANICAL PROPERTIES AND IRRADIATION DAMAGE NUCLEATION OF HTGR GRAPHITES — $ 38,200 — 01-4
P. A. Thrower - Dept. of Materials Science
Phone: (814)-865-1934

Degradation of graphite by water vapor, air, and mixtures of CO and CO_2; effect of various filler: binder ratios and porosity characteristics; residual strength measurements; TEM examination of neutron irradiated pyrolytic graphite.

PENNSYLVANIA STATE UNIVERSITY (Continued)

385. STRUCTURE OF GLASSES CONTAINING TRANSITION METAL IONS — $ 72,000 — 01-1

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

Structure and stability of insulator glasses with transition metal oxide additions; degree of order, structure of modifier; transition metal sites; theory of crystal field effects and electronic transitions in glass environment; glass structure relative to crystals of same composition; phase separation; leaching, dipole derivatives; bond character, Raman and infrared spectroscopy, optical absorption, luminescence, X-ray diffraction and electron microscopy; silicate, borate, borosilicate, germanate and phosphate glasses with Zn, Cr, Fe, Mn and Ni additions, alkali-alumina-silica and high silica alkali silicate glasses.

UNIVERSITY OF PENNSYLVANIA

386. ELECTROCHEMICAL INVESTIGATION OF NOVEL ELECTRODE MATERIALS — $ 75,000 — 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.

UNIVERSITY OF PITTSBURGH

387. STUDIES FOR THE PRODUCTION OF SUPER-PURE SILICON NITRIDE — $ 45,000 — 03-3

P. E. D. Morgan - Dept. of Metallurgical and Materials Engineering
Phone: (412)-624-5300

Synthesis of pure amorphous silicon nitride by three techniques: Sulfur catalyzing the nitriding of ultra-pure silicon, silicon nitride synthesis from silicon tetrachloride and powdered silicon nitriding in a plasma glow discharge to produce the amorphous form from atomic nitrogen at low temperatures.

PRINCETON UNIVERSITY

388. CHEMICAL POISONING IN HETEROGENEOUSLY CATALYZED REACTIONS — $ 48,000 — 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

389. HIGH TEMPERATURE EFFECTS OF INTERNAL GAS PRESSURES IN CERAMICS — $ 59,440 — 01-3

A. A. Solomon - Dept. of Nuclear Engineering
Phone: (317)-494-6151

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.

RENSSELAER POLYTECHNIC INSTITUTE

390. LOCALIZED CORROSION AND STRESS CORROSION CRACKING BEHAVIOR OF AUSTENITIC STAINLESS STEEL WELDMENTS CONTAINING RETAINED FERRITE — $ 72,000 — 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; stress corrosion cracking studied at slow strain rates in pressure vessels with electrochemical monitoring of potentials.

RENSSELAER POLYTECHNIC INSTITUTE (Continued)

391. FATIGUE BEHAVIOR OF BCC METALS — $ 43,600 — 01-2
N. S. Stoloff - Dept. of Materials Engineering
Phone: (518)-270-6495

Fatigue behavior of bcc metal-hydrogen alloys; effects of microstructural, testing and environmental factors; high cycle (stress-controlled) and low cycle (strain-controlled) conditions; dislocation substructure and hydride phase effects; room and elevated temperatures; transmission electron microscopy; V, Nb, V-H and Nb-H alloys.

392. CHEMICAL DIFFUSION ON SOLID SURFACES — $ 24,600 — 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 — 01-2

393. 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 — $ 37,625
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; nondestructive evaluation.

UNIVERSITY OF ROCHESTER

394. THE MATERIALS AND MECHANICS OF RATE EFFECTS IN BRITTLE FRACTURE — $ 55,000 — 01-2
S. J. Burns - Dept. of Mechanical and Aerospace Science
Phone: (716)-275-4082

Slow, steady state crack propagation in PMMA; crack velocity, crack extension force and specimen temperature varied over a wide range and analyzed in the formalism of thermally activated crack propagation; rapid crack propagation data in steels analyzed assuming adiabatic crack propagation; multiple test specimens that differ only in crack area to be tested to determine the crack extension force when the crack starts to propagate.

UNIVERSITY OF ROCHESTER (Continued)

395. DIFFUSIONAL CREEP OF MULTI-COMPONENT SYSTEMS — $ 70,190 — 01-2
J. C. M. Li - Dept. of Mechanical and Aerospace Sciences
Phone: (716)-275-4038

Impression creep studies on Cu-Ni single crystals of various compositions and on beta-Sn single crystals of three orientations; tests to be extended to the Bi-Sb system; micro-impression elasticity to measure local elastic modulus using the indentation technique; impression creep studies to be extended to low temperatures; creep mechanisms by selective laser excitation.

ROCKWELL INTERNATIONAL

396. ACOUSTIC EMISSION SIGNATURE ANALYSIS — $ 94,147 — 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.

397. SINTERING PHENOMENA OF NON-OXIDE SILICON COMPOUNDS — $ 69,998
F. F. Lange - Science Center
Phone: (805)-498-4545
D. R. Clarke - Science Center
Phone: (805)-498-4545

Sintering of non-oxide silicon compounds; volatilization phenomena; liquid phase sintering; grain boundary grooving; transmission electron microscopy, lattice fringe imaging.

UNIVERSITY OF SOUTHERN CALIFORNIA

398. ELECTRICAL AND MECHANICAL PROPERTIES OF OXIDE CERAMICS — $ 57,800 — 01-3
F. A. Kroger - 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; rate-controlling defect species; concentration and thermodynamics, separation of bulk and grain boundary effects; sintering; hot pressing; Auger electron spectroscopy; thermal grooving; polycrystalline Al_2O_3, pure and doped with Fe, Mg, Ti, or Co.

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

Measurement of grain boundary sliding and cavitation in creep of Al and Mg alloys; deformation mechanisms related to creep-rupture behavior; grain size effects; deformation maps; diffusion and dislocation controlled creep in alkali-halides and oxides.

400. EVAPORATION DRIVEN LIQUID SINTERING — $ 53,900 — 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.

401. CHEMISTRY OF ZIRCONIUM RELATED TO THE BEHAVIOR OF NUCLEAR REACTOR FUEL CLADDING — $ 75,000 — 03-3
D. Cubicciotti - Dept. of Chemistry
Phone: (415)-326-6200, X3940

Thermodynamics of solid and gaseous zirconium iodides. Kinetics of iodide film growth on zirconium surfaces, kinetics of oxidation of zirconium under low oxygen activity, physical and chemical mechanisms of oxide film disruption, and formation of compounds of zirconium and other elements in the fuel-cladding gap.

STANFORD UNIVERSITY

402. PHOTOVOLTAIC MATERIALS RESEARCH- II-VI HETEROJUNCTIONS AND Cu_2S/CdS THIN FILMS — $121,129 — 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; microdiffraction; vacuum evaporation; spray pyrolysis; rf sputter deposition.

403. SUPERCONDUCTING AND SEMICONDUCTING PROPERTIES OF ELECTRON BEAM EVAPORATED MATERIALS — $ 86,400 — 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 co-evaporation 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.

404. MODELING OF DEFORMATION AND FRACTURE IN HIGH-TEMPERATURE STRUCTURAL MATERIALS — $ 98,000 — 01-2

A. K. Miller - Dept. of Materials Sciences
Phone: (415)-497-2536
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 stainless steel; kinematic hardening during cyclic deformation; design of high-strain reversed torsion apparatus; steady state flow at intermediate temperatures in Al; application of constitutive equations to fracture; transient subgrain refinement strengthening.

STANFORD UNIVERSITY (Continued)

405. STRUCTURE DEPENDENCE OF HIGH TEMPERATURE DEFORMATION OF METALS — $ 74,800 — 01-2
W. D. Nix - Dept. of Materials Science and Engineering
Phone: (415)-497-4259

Experimental and analytical evaluation of creep-rupture behavior of metals; cavity growth and coalescence, and intercavity ligament yielding in Ag and Cu embrittled by H_2O bubbles at grain boundaries; creep models based on dislocation core diffusion controlled climb or on grain boundary diffusion; effect of Al_2O_3 despersoid on twinning and dislocation motion during creep of fine-grained Ni; influence of segregation of P on creep of Fe-base alloys.

406. DIFFUSION OF OXYGEN IN LIQUID METAL SYSTEMS — $ 49,640 — 01-3
D. A. Stevenson - Dept. of Materials Science
Phone: (415)-497-4251

Oxygen solubility, thermodynamic activity and diffusion in liquid metal alloy solutions; solute-solute interaction studies, calorimetric titration and time dependent currents using oxygen ion conducting solid electrolytes; aging of solid oxide electrolytes; transference numbers by AC techniques; Y_2O_3-doped ThO_2 electrolytes; Ga-In-O, Sb-Bi-O, and In-Ca, Ag, etc. systems.

SYRACUSE UNIVERSITY

407. SURFACE CHARACTERIZATION OF CATALYTICALLY ACTIVE METAL ALLOY AND COMPOUND FILMS — $ 83,400 — 01-1
R. W. Vook - Chemical Engineering and Materials Science Dept.
Phone: (315)-423-3466

Correlation of surface structure with catalytic activity of Pt and Pd in CO oxidation; influence of overlayer morphology, defect structure, and elastic strain; techniques used: AES, TEM, RHEED.

UNIVERSITY OF TENNESSEE

408. A COMBINED THERMODYNAMIC STUDY OF NICKEL-BASE ALLOYS — $ 70,000 — 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 TEXAS

409. SYNTHESIS OF NEW FUNCTIONALIZED FLUOROCARBON POLYMERS FOR USE AS BATTERY SEPARATORS AND MEMBRANES — $ 83,000 — 03-2

R. J. Lagow - Dept. of Chemistry
Phone: (512)-471-1032

Synthesis of polymers by oxyfluorination to convert the thermal methyl in pendant groups to acid fluorides which functionalize the polymer and act as sites for further membrane chemistry. Conversion of thin polymer films completely to fluorocarbon material and polymer powders by a two-step process to membranes and separators.

U. S. STEEL CORPORATION

410. STUDIES OF FUNDAMENTAL FACTORS CONTROLLING CATALYZATION OF REACTIONS OF GASES WITH CARBONACEOUS SOLIDS — $ 67,940 — 01-1

R. M. Fisher - Research Laboratory
Phone: (412)-351-3100, X2904

Metal particle catalyzed gasification of carbon; effect of particle size and number; effect of particle alloy composition; in-situ scanning and transmission electron microscopy; Fe particles on graphite.

UNIVERSITY OF UTAH

411. IMPURITY EFFECTS ON THE CREEP OF POLYCRYSTALLINE MAGNESIUM AND ALUMINUM OXIDES AT ELEVATED TEMPERATURES — $ 43,000 — 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.

412. ELECTROLYTIC DEGRADATION OF LITHIA-STABILIZED β" ALUMINA — $ 63,000 — 03-2

D. K. Shetty - Dept. of Materials Science and Engineering
Phone: (801)-581-5604
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.

VARIAN ASSOCIATES

413. RESEARCH ON LATTICE MISMATCHED SEMICONDUCTOR LAYERS — $ 92,941 — 01-3

R. L. Bell - Solid State Laboratory
Phone: (415)-493-4000, X2906
R. L. Moon - Solid State Laboratory
Phone: (415)-493-4000, X3278

Morphology and properties of semiconducting III-V compound ternary, quaternary and quinary epitaxial layers grown lattice-mismatched on substrates with reference to their ultimate applications in high efficiency solar cells; characteristics of materials grown by the liquid phase melt depletion lattice parameter grading method; AlGaAsSb and GaAsP 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

414. HYDROGEN EMBRITTLEMENT TESTING — $ 32,000 — 01-2
M. R. Louthan, Jr. - Dept. of Materials Engineering
Phone: (703)-951-6825

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 WISCONSIN — $ 75,000 — 01-4

415. VOID NUCLEATION AND GROWTH IN HEAVY ION AND ELECTRON BOMBARDED PURE METALS
G. L. Kulcinski - Dept. of Nuclear Engineering
Phone: (608)-263-2308
P. Wilkes - Dept. of Nuclear Engineering
Phone: (608)-263-2196

Effects of irradiation variables and material parameters influencing void formation in metals; dilatometric studies of irradiation damage annealing; heavy ion and electron simulation of neutron irradiating effects of temperature, fluence, flux and interstitial impurities; swelling; high voltage electron microscopy; 18 MeV copper bombardment of V and V-N alloys; 1 MeV electron bombardment of Al.

416. LOCAL ELECTRONIC PROPERTIES OF SEMICONDUCTOR SURFACES AND INTERFACES — $ 71,660 — 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.

UNIVERSITY OF WISCONSIN (Continued)

417. PREDICTION OF THE BEHAVIOR OF STRUCTURAL MATERIALS UNDER IRRADIATION THROUGH MODELLING OF THE MICROSTRUCTURE — $ 34,900 — 01-4

W. G. Wolfer, Dept. of Nuclear Engineering
Phone: (608)-263-1646

Modelling of nucleation and growth of radiation-induced voids and dislocations; effect of spatial correlations between sinks for point defects and time dependence of their production.

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, 1978, the Materials Sciences total support level amounted to about $59.7 million in operating funds (budget outlays) and $5.1 million in equipment funds. The equipment funds are expended primarily at Laboratories and are not shown in this report. 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 (%)	Total Program (%)
(a) Northeast..... (Mass., Penn., N.Y., D.C., Md., Vt., Conn., N.H., R.I.)	43.9	18.0
(b) South..... (Fla., N.C., Tenn., Va., Georgia)	6.7	23.5
(c) Midwest..... (Ohio, Ill., Wisc., Mich., Minn., Ind., Iowa, Kan.)	19.7	37.7
(d) West..... (Ariz., Okla., Wash., Texas, Hawaii, N. Mex., Calif., Utah, Colo., Idaho)	29.7	20.8
	100.0	100.0

2. By Academic Department or Laboratory Division:

	Contract Research (%)	Total Program (%)
(a) Metallurgy, Materials Science, Ceramics (Office Budget Activity Numbers 01-).....	61.0	43.0

	Contract Research (%)	Total Program (%)
(b) Physics, Solid State Science, Solid State Physics (Office Budget Activity Numbers 02-)....	30.4	42.1
(c) Chemistry, Chemical Eng. (Office Budget Activity Numbers 03-).....	8.6	14.9
	100.0	100.0

3. By DOE Laboratory and University:

	Total Program (%)
(a) University Program (including those laboratories where graduate students are involved in research to a large extent, e.g., LBL, Ames).....	35.9%
(b) Laboratory Program.....	64.1%
	100.0%

4. By Laboratory:

	Total Program (%)
Ames Laboratory.....	9.5
Argonne National Laboratory.....	21.7
Brookhaven National Laboratory.....	10.9
Idaho National Engineering Laboratory.....	0.5
Illinois, University of (Materials Research Laboratory).....	3.0
Lawrence Berkeley Laboratory.....	7.5
Lawrence Livermore Laboratory.....	1.7
Los Alamos Scientific Laboratory.....	2.0
Mound Laboratory.....	0.2
Oak Ridge National Laboratory.....	22.6
Pacific Northwest Laboratory.....	2.5
Sandia Laboratory.....	2.0
Contract Research.....	15.9
	100.0

5. By Selected Areas of Research:

	Number of Projects (Total=345) (%)	Total Program $ (%)
(a) Materials		
Polymers	4.1	1.5
Ceramics	23.1	16.0
Semiconductors	9.6	6.4
Hydrides	8.1	4.1
Ferrous Metals	12.8	8.3
(b) Technique		
Neutron Scattering	6.1	14.5
Theory	11.6	8.6
(c) Phenomena		
Catalysis	7.8	5.0
Corrosion	6.1	3.5
Diffusion	8.7	5.1
Superconductivity	9.0	8.9
Strength	16.6	10.2
(d) Environment		
Radiation	9.9	13.6

SECTION D

Index of Investigators, Materials, Phenomena, Technique and Environment

The index refers to project numbers in Sections A & B.

Actinide Metals and Compounds

Ceramics

Carbides

Glass

Nitrides

Oxides

Composites

10
89
137
141
335
350

Fast Ion Conductors

51
59
70
97
103
117
120
126
190
196
206
312
376

Graphite, Carbon, and Coal

14
31
34
40
80
97
111
141
157
175
178
204
209
320
322
351
384
410

Hydrides

5
24
30
41
42
49
50
52
59
60
66
74
75
80
91
112
120
123
124
170
190
305
318
336
347
349
368
391

Intermetallic Compounds

32	132	403
45	137	
49	184	
53	188	
64	189	
66	191	
70	214	
89	310	
105	321	

Ionic Crystals

26	70
30	73
60	98
61	101
62	

Liquids & Amorphous Materials

15	77	105	204	313
26	81	135	206	320
35	82	145	222	327
36	83	160	223	331
59	86	163	302	406
60	90	167	304	
68	94	173	311	

Metals

Alkali

77
79
85
169
173
324
386

BCC Refractory

2	111	349
5	112	375
10	124	391
11	126	393
18	180	415
20	181	
24	190	
25	198	
26	215	
32	318	
33	332	
37	336	
49	340	
77	343	

Ferrous

2	186	341
15	188	354
47	193	357
55	195	362
58	199	363
77	207	373
88	212	375
89	213	379
130	221	380
132	222	390
159	303	396
168	317	404
179	324	405
181	332	414
185	336	

MHD Materials

44
71
85
103
115

Polymers

26	204
113	306
114	342
119	350
122	394
161	409
175	
188	

Rare Earth Metals and Compounds

1	27	84
3	30	117
9	32	188
11	44	189
13	61	197
22	74	347
23	80	

Semiconductors

1	135	222
26	145	226
27	146	302
28	147	308
52	149	334
61	193	338
68	194	374
70	197	402
90	200	413
111	203	416
121	210	
129	211	

Acoustic Emission

396

Auger Electron Spectroscopy

181
202
212
224
307
347
355
363
392
398
407
416

Computer Simulation

12
19
48
70
85
100
134
197
319
404

Elastic Constants

49
124
347
370
393

Electron Microscopy

5
6
18
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Electron Spin Resonance

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69
117
192
312
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Field Emission and Ion Microscopy

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54
224
225
332

High Temperature Heat Capacity

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76
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Infrared Spectroscopy

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107 320
135 385
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53 200
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55 222
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Neutron Scattering

Nondestructive Evaluation

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40	312
50	376
51	
63	
65	
113	
119	
127	
157	

Optical Spectroscopy

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27	210
36	218
67	302
68	365
82	370
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135	
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Positron Annihilation

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Sputtering

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Theory

Thermal Conductivity

Thermodynamics

X-Ray Photoelectron Spectroscopy

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X-Ray Scattering

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Catalysis

Corrosion

Crystal Structure, Atomic Distribution and Crystal Transformations

Diffusion

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5	192	392
8	197	395
38	206	406
51	222	
76	228	
112	314	
116	326	
126	350	
152	355	
154	356	
155	358	
169	383	

Dislocations

18	338
48	344
118	372
124	375
174	
199	
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Erosion

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109
142
143
177
223

Electron and Ion Conduction

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44	305
69	319
116	326
119	334
141	358
152	360
192	371
196	376
206	398
226	

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Magnetism

Materials Preparation and Characterization

Phonons

Photovoltaic and Photothermal Phenomena

Point Defects

Precipitation

Recovery and Recrystallization

Sintering

Solidification

Strength

Fracture

Constitutive Equations

Fatigue

Creep

Flow Stress

Stress-Corrosion Cracking

Superconductivity

Surface Phenomena and Thin Films

Welding

Gas

Oxidizing

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Hydrogen

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Sulphur-Containing

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182
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Magnetic Field

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127
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189
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Pressure

Above Atmospheric

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122
126
151
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Radiation

Electron

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54
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129
131
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375
415

Ion

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Neutron

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Photons

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Theory

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Gamma

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Temperature

Very Low Temperatures

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High Temperatures

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