ERDA-77-123

Materials Sciences Programs

Energy Research and Development Administration

Division of Basic Energy Sciences

FY 1977

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FOREWORD

During FY 1977 a new Department of Energy was proposed by the President and approved by Congress. This Department is now (August, 1977) scheduled for activation about October 1, 1977. The Energy Research and Development Administration will be transferred to the Department of Energy together with other agencies and parts of agencies within the Federal government. Also during FY 1977 the Division of Physical Research of ERDA was reorganized into two Divisions, one called Basic Energy Sciences and one called High Energy and Nuclear Physics. At the time of this writing the organizational structure of the new Department of Energy has been established only at the functional levels. However, it is expected that the Divisions of Basic Energy Sciences and High Energy and Nuclear Physics will report to the Director of the D.O.E. Office of Energy Research. The Director of this Office will be appointed by the President with Senate consent. The Director shall advise the Secretary on the physical research program transferred to the Department from ERDA; monitor the Department's R&D programs; advise 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 advise the Secretary on basic and applied research activities of the Department.

The Materials Sciences Subprogram constitutes one portion of a wide range of research supported by the ERDA Division of Basic Energy Sciences. Other programs are administered by the Division's Chemical Sciences, Nuclear Sciences, Engineering, Mathematical and Geoscience Sciences, and Advanced Energy Projects Offices. Materials Sciences research is supported primarily at ERDA National Laboratories and Universities. The research covers a spectrum of scientific and engineering areas of interest to the Energy Research and Development Administration and is conducted generally by personnel trained in the disciplines of Solid State Physics, Metallurgy, Ceramics and Chemistry. The structure of the Office is given in an accompanying chart.

The Materials Sciences Subprogram 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 under way in FY 1977 together with a convenient index to the program.

Donald K. Stevens
Assistant Director
(for Materials Sciences Program)
Division of Basic Energy Sciences

INTRODUCTION

The purpose of this report is to provide a convenient compilation and index of ERDA's Materials Sciences Program. 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.

Each project carries a number (underlined) for reference purposes. The FY 1976 funding level, title, personnel, budget activity number (e.g. 01-02), 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:

01-01 - Structure of Materials
01-02 - Mechanical Properties
01-03 - Physical Properties
01-04 - Radiation Effects
01-05 - Engineering Materials (to start FY 1978)

02-01 - Neutron Scattering
02-02 - Experimental Research
02-03 - Theoretical Research
02-04 - Particle-Solid Interactions
02-05 - Engineering Physics (to start FY 1978)

03-01 - Chemical Structure
03-02 - Engineering Chemistry
03-03 - 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.

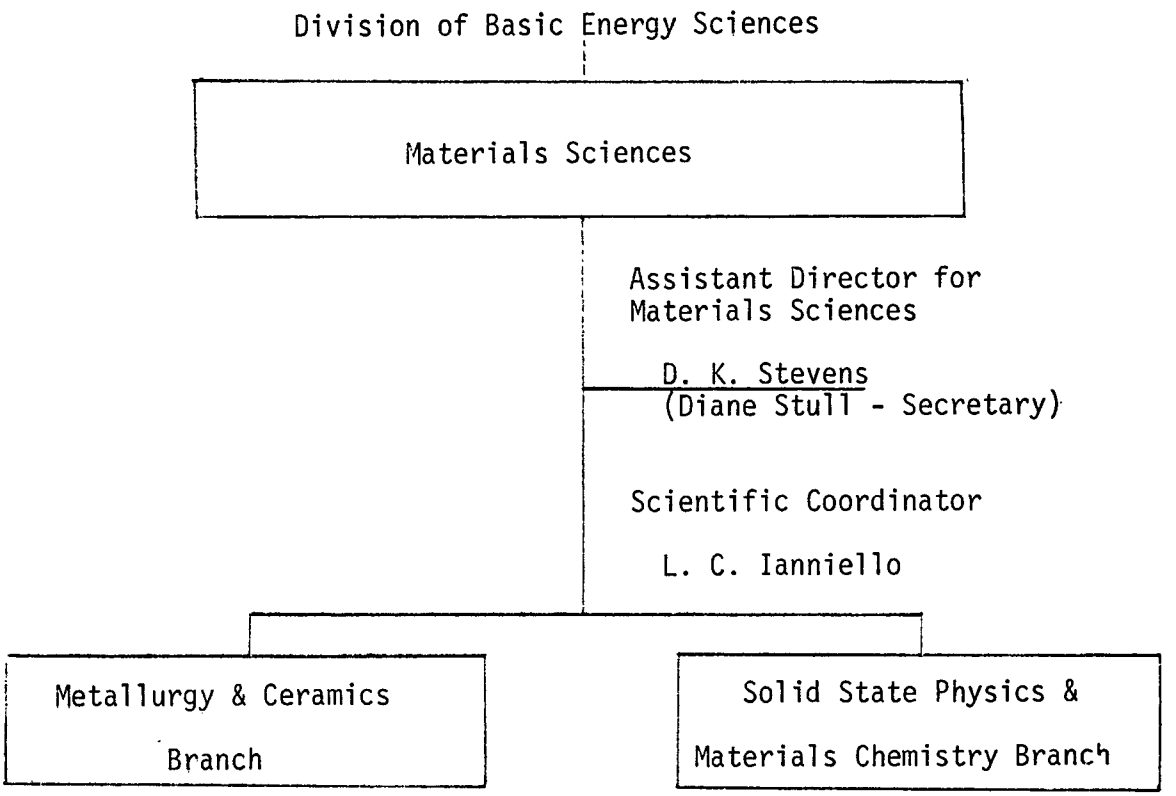
It should be recognized that it is impossible to include in this report all the technical data available for such a large program. By the time it could be compiled it would be outdated. The approach taken here was to summarize each project with key words and phrases reflecting the activity under the project. The best method for obtaining more detailed information about a given research project is to contact directly the investigators listed.

Louis C. Ianniello
Materials Sciences Program
Division of Physical Research

STRUCTURE

OF

MATERIALS SCIENCES OFFICE



Notes:
1/ Address as of 9/77, Ohio State University
2/ Returned to Purdue University - 8/77
3/ To start 9/77
4/ On Year's Leave from Pacific Northwest Laboratory - Starting 9/77
5/ On Leave from Georgetown University

Date: August 26, 1977

TABLE OF CONTENTS

SECTION A - Laboratories

	Page
Ames Laboratory	1
Argonne National Laboratory	13
Brookhaven National Laboratory	29
Idaho National Engineering Laboratory	34
Illinois, University of	35
Lawrence Berkeley Laboratory	39
Lawrence Livermore Laboratory	48
Los Alamos Scientific Laboratory	50
Mound Laboratory	52
Oak Ridge National Laboratory	53
Pacific Northwest Laboratory	66
Sandia, Albuquerque	69
Sandia, Livermore	71

SECTION B - Universities

Alphabetical Listing 74-100

SECTION C - Funding Levels

Region	102
Department	102
Laboratory versus University	103
Laboratories	103
Reserach Area	104

SECTION D - Index

Investigators	A1
Materials	A9
Technique	A13
Phenomena	A19
Environment	A25

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 1977.

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

STRUCTURE OF MATERIALS $400,000 01-01

1. MASS TRANSPORT
O. N. Carlson, F. A. Schmidt

Electrotransport studies of Fe, Co and Ni in α and β Th; determination of diffusivities, migration velocities and effective valences. Study of electrotransport of Fe and Al in Si and of C, N and O in La. Thermotransport studies of solutes in refractory metals and alloys; study of migration behavior and heat of transport (Q*) for C, N, and O in V and V-Ti alloys.

2. SEMICONDUCTING AND THERMOELECTRIC MATERIALS
F. A. Schmidt, R. K. Trivedi
D. E. Williams

Growth of semiconducting crystals from dendritic seeds, Dendritic web technique; experimental and theoretical studies of dendrite-melt interface kinetics and growth/pull rate relationships for Si and Ge. Deposition of thin films of semiconducting materials on mechanically suitable metal substrates; bonding, interface characterization, and work function studies involving Si on W and Pt.

3. HIGH PURITY METALS
B. J. Beaudry, K. A. Gschneidner, Jr.

Preparation of high purity rare earth metals, refractory metals, thorium and silicon. Study of the effects of interstitial impurities on the properties of metals. Preparation of high purity mischmetal. Growth of oriented single crystals of rare earth compounds and solid solutions. Development of methods for controlling optical, thermal and electrical properties of rare earth-sulfur compounds through the variation of sulfur content.

AMES LABORATORY
Metallurgy and Ceramics -01- (Continued)

4. IMPROVED STRUCTURE AND STABILITY OF HIGH TEMPERATURE ALLOYS
O. N. Carlson, R. K. Trivedi

Study of the solution strengthening of ferritic alloys; determination of the solubility limits of the Chi-phase, $Fe_{36}\ Cr_{12}\ Mo_{10-x}\ Ti_x$, in the alpha phase of these four components over the temperature range 700 to 1250°C. Determination of the effects of Chi-phase stoichiometry changes on its physical and mechanical properties. Surface diffusion studies of vanadium at high temperatures. Correlation of diffusion characteristics with impurity segregation which is believed to exist near the surface and on certain crystallographic faces of vanadium.

MECHANICAL PROPERTIES $430,000 01-01

5. CERAMICS
O. Hunter

Control of microcracking in sintered monoclinic Eu_2O_3 by additions of grain growth inhibitor, Ta_2O_5. Study of microcracking tendencies of hot-pressed HfO_2 as a function of grain size and the alteration of the crystal structure of HfO_2 through the addition of a second oxide, e.g., Y_2O_3, to improve the mechanical properties. Determination of the thermal expansion, thermal diffusivity and elastic properties of Y_2O_3 doped HfO_2 and other ceramics which have potential application as MHD channel materials.

6. INFLUENCE OF HYDROGEN ON MECHANICAL PROPERTIES OF METALS
T. E. Scott

Study of the hydrogen embrittlement mechanisms operating in the refractory metals, V, Nb, and Ta; effect of oxygen and carbon doping on embrittlement and hydride formation, effects of stress on reorientation of hydrides in metals, study of embrittlement kinetics. Studies of the effects of stress state and various impurity gases, (e.g., H_2S, CH_4, CO, CO_2) on the hydrogen attack of steels.

AMES LABORATORY
Metallurgy and Ceramics -01- (Continued)

7. HYDROGEN TRANSPORT AND DIFFUSION STUDIES
D. T. Peterson

Thermotransport studies of hydrogen and deuterium in Nb and Ta including measurements of the heat of transport Q* and the ratio of Q^*_H/Q^*_D. Electrotransport measurements of hydrogen and deuterium in Nb-Ta alloys; variation of Z* (effective change) is being studied with changes in hydrogen concentration and temperature. Measurement of diffusion coefficients for hydrogen in Ta, Nb and Nb-Ta alloys.

8. PURIFICATION BY EXTERNAL GETTERING
D. T. Peterson

Development of a method for the removal of interstitial impurities from V through the outward diffusion and consequent reaction of the impurities with a thin layer of Ti applied to outer surface; application of Ti gettering method to the production of high purity single cyrstals.

9. STRESS CORROSION CRACKING STUDIES
T. E. Scott

Investigation of the mechanism of stress corrosion cracking; a study of the effects of deformation on the phenomenon and a characterization of the near-surface dislocation structure. (An interdisciplinary study with Solid State Physics).

PHYSICAL PROPERTIES $790,000 01-03

10. CERAMICS
M. F. Berard, D. R. Wilder

Thermal diffusion studies in ceramic systems; gradients up to 300°C/cm and temperatures up to 1400°C can be maintained, SrF_2-CaF_2 and YF_3-CaF_2 solid solutions are being studied. Other diffusion studies in ceramic systems include Hf and Er in Er_2O_3, Ca in YF_3-doped CaF_2, and Ca, Sr and Ba in pure CaF_2 and SrF_2. Determination of the complete phase diagram for the HfO_2-Eu_2O_3 system and the correlation of phase equilibrium data with sintering characteristics of HfO_2. Metal-ceramic interface studies; exploration of metal ductility enhancement resulting from metal-ceramic reactions at the interface. Study of thermal and mechanical properties of several ceramics with potential applications in MHD systems.

AMES LABORATORY
Metallurgy and Ceramics -01- (Continued)

11. ELECTRICAL AND MAGNETIC BEHAVIOR
C. W. Chen, K. A. Gschneidner, Jr.,
O. D. McMasters, J. W. Patterson,
J. F.Smith, J. D. Verhoeven

Magnetic susceptibility measurements on Th, Th-C alloys, MnPt and Mn-Pt alloys, and rare earth-rich solid solutions. The influence of impurities (Fe, Zr and Mg) on the heat capacity and other physical properties of Sc and Ce is being studied. Development of electron bombarded LaB_6 cathode design for electron sources and electron optical devices; elimination of radiant heating of LaB_6 rod reduces power consumption and prolongs cathode life. Solid electrolyte studies; electrical conductivity and EMF measurements are being conducted on YOF to elucidate the electrical and ionic characteristics of this material in both its high and low temperature forms. Preparation of large single crystals of solid solutions and intermetallic compounds by induction levitation technique; crystals of rare earths and intra-rare earth alloys are being prepared for electrical and magnetic property studies.

12. ELASTIC CONSTANT STUDIES
J. F. Smith

Development of nondestructive method for determination of large bolt tension (and, hence, optimum tightness) by ultrasonic measurement of elastic constants; applicable to pressure vessels, large machinery, etc. Study of the effects of H on the elastic properties of Nb and Nb-H alloys.

13. SUPERCONDUCTIVITY
K. A. Gschneidner, Jr., J. D. Verhoeven

Low temperature, high magnetic field heat capacity studies of 4f - type superconductors, La_3In, $LaOs_2$ and La_3S_4. Preparation of superconducting composite materials by directional solidification.

14. ALIGNED COMPOSITE MATERIALS
J. D. Verhoeven

Study of the factors controlling the growth of aligned composite materials by directional solidification and directional transformation; high strength materials and superconductors may be prepared by these methods.

AMES LABORATORY
Metallurgy and Ceramics -01- (Continued)

15. HIGH TEMPERATURE - CORROSION RESISTANT MATERIALS
F. X. Kayser

Single crystal preparation and physical property measurement of Ni_3Al; corrosion resistance and high temperature strength of the material are being determined. Physical properties and corrosion resistance studies of Fe_3Al:Fe_3Si, a long range ordered solid solution. Extensive studies on other long range ordered systems including Si-Fe and Cu-Au alloys. Production of rare earth coatings for improved oxidation resistance; the effects of valence and atomic size are being evaluated.

16. ALLOY THEORY, THERMODYNAMIC, AND PHASE STABILITY STUDIES
D. M. Bailey, P. Chiotti, J. F. Smith

Development of methods for the calculation of phase diagrams and prediction of phase stabilities in multicomponent systems from thermodynamic data. Thermodynamic studies of mixed double oxides and the correlation of these results with corrosion of Fe-Cr-Ni alloys by oxygen containing liquid sodium.

17. RADIATION EFFECTS $280,000 01-04
C. W. Chen, M. S. Wechsler

Studies of the clustering of radiation-induced point defects in Nb and V and of the effects of annealing on these defect clusters. Annealing studies of irradiated BCC metals and considerations of the effects of impurities upon the observed annealing behavior. Characterization of the recovery mechanisms operating in neutron-irradiated and cold-worked Th. Determination of the effects of irradiation on the mechanical properties of Th and Th-C alloys. Evaluation of the effectiveness of dopants on the suppression of void formation in irradiated BCC metals.

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

18. NEUTRON SCATTERING $560,000 02-01
W. A. Kamitakahara, J. Khatamian,
G. R. Kline, C. Stassis,
A. S. Edelstein

Study of the dynamical characteristics of solids at high temperatures, including phonon properties, bonding, melting, and structural phase transitions (Zr, Ti); effect of hydrogen and carbon impurities in metals (Th-C); electron-phonon interaction and its relation to superconductivity (Zr_2Ni, La_3S_4); electronic distributions in transition metals, rare earth metals, and mixed-valence compounds (Ce, Zr, $CeSn_3$).

19. MAGNETIC PROPERTIES OF SOLIDS $ 50,800 02-02
S. Legvold

Magnetic and transport properties of localized and conduction band (itinerant) electrons in rare earth metals and alloys; correlations between magnetic ordering temperatures of alloys and their residual resistivities (Tb-Sc, Tb-Y, Tb-La, etc.); magnetic ordering in Nb-La and Ce-La alloys; Cooper-pair breaking in superconducting La containing magnetic impurities (La-Tb, La-Dy, La-Ho, etc.); magnetic and crystal field effects in La alloys (La-Sm, La-Ce); electrical resistivity of single crystal La; Seebeck effect in alloys at low temperatures (Y-Ce, Ce-La, Nd-La).

20. NUCLEAR RESONANCE IN SOLIDS $208,400 02-02
R. G. Barnes, Y. S. Hwang,
D. R. Torgeson

Applications of nuclear magnetic resonance, nuclear quadrupole resonance, and Mössbauer 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); characterization of lattice perfection and structural transformations in superconducting intermetallic compounds (e.g., $NbSe_2$, HfV_2); charge density wave effects in superconducting intermetallic compounds (e.g., $NbSe_2$, $TaSe_2$); electronic structure of one and two-dimensional metals (e.g., ZrCl, Sc_7Cl_{10}).

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

21. OPTICAL AND SPECTROSCOPIC PROPERTIES OF SOLIDS AND LIQUIDS — $174,500 — 02-02
T. E. Furtak, A. Habenschuss, D. W. Lynch, C. G. Olson, F. H. Spedding, R. Rosei, J. H. Weaver

Optical properties (transmission, reflection, thermoreflection, electroreflection) of solids in the near infrared, visible, and vacuum ultraviolet (using synchrotron radiation): transition metal alloys and compounds (e.g., FeTi), transition metal-hydrogen systems, noble metals, III-V, IV, and II-VI semiconductors. Photoemission into liquid electrolytes, electrochemical modulation spectroscopy, microspectroelectrochemistry, and photoelectrochemistry: binary alloys susceptible to localized corrosion, surface excitation, and adsorption phenomena. 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.

22. THERMODYNAMIC AND TRANSPORT PROPERTIES OF SOLIDS — $381,500 — 02-02
M. S. Anderson, A. J. Bevolo, G. C. Danielson, D. E. Eckels, H. R. Shanks, C. A. Swenson

Electrocatalytic activity of tungsten bronzes (Na_xWO_3); electrical resistivity, thermal conductivity, and Seebeck coefficient of high purity vanadium and tantalum; heat capacity of Pb-Cd layer composites; 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; precision thermometry and temperature scales; 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); photolysis using thin-film corrosion-resistant coatings to prevent decomposition of the semiconducting electrodes. 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); passivation layers on rare earths; corrosion of surfaces; evaporated and sputtered thin films, Schottky-barrier, and metal-oxide-semiconductor interfaces; backwall Schottky-barrier solar cells; amorphous silicon-metal interfaces; ohmic contacts to silicon; compositional variation in superconductor-normal metal composites.

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

23. SUPERCONDUCTIVITY $254,800 02-02
D. K. Finnemore, T. Y. Hsiang, P. S. Martinoli, J. W. Osmun, J. E. Ostenson, E. L. Wolf, M. Zaitlin, R. E. Noer

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 at Pb-Cd superconductor-normal metal boundaries; Josephson tunneling and coherent flux motion in granular aluminum spatially modulated superconductors. Auger analysis and photoemission of getter sputtered and surface grown V_3Ga and other A-15 superconducting films.

24. MAGNETIC AND ELECTRONIC PROPERTIES OF SOLIDS THEORY $141,500 02-03
B. N. Harmon, S. H. Liu

Electronic properties of transition metals and compounds (CrB_2, ZrB_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.

25. SUPERCONDUCTIVITY THEORY $ 43,200 02-03
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, optical and transport properties of highly anisotropic systems; new mechanisms for superconductivity in linear conductors.

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

26.	OPTICAL AND SURFACE PHYSICS THEORY R. Fuchs, K. L. Kliewer, J. Reyes, P. R. Rimbey, P. Halevi	$145,300	02-03

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. 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-charge materials for solar applications.

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

27. X-RAY AND NEUTRON CRYSTALLOGRAPHY — $256,000 — 03-01
R. A. Jacobson, J. E. Benson
B. J. Helland

Development of diffraction techniques, structural methods in the solid state, intercalated transition metal dichalcogenides, metal complexes, intramolecular solid-state interactions, mineral content of coal, coal characterization.

28. LOW OXIDATION STATES IN INORGANIC SYSTEMS — $157,500 — 03-01
J. D. Corbett, H. Imoto

Preparation and characterization of new types of inorganic materials under anaerobic, high temperature, and reducing conditions (e.g., for Sc, Ti, Zr, Hf, Mo, rare earths); structures exhibiting extended metal-metal bonding; homopolyatomic ions (e.g., of Sn, Sb, Pb, Bi, Te); ionic intermetallic phases.

29. CHEMISTRY OF HEAVY TRANSITION METALS — $116,500 — 03-01
R. E. McCarley, M. S. Matson

Chemistry of heavy transition elements, especially Nb, Ta, Mo, W; preparation and characterization of dimeric and cluster compounds with strong metal-metal bonds; properties and reactions of metal cluster compounds with potential for energy storage and catalytic applications; compounds with unusual reactivity.

30. LIQUID METALS — $ 52,000 — 03-02
R. G. Bautista, G. Burnet

Heat capacities and heat content of liquid binary alloy (Cu-Ce) and low melting point eutectic mixtures containing yttrium, lanthanum or cerium; characterization of gases in liquid metal alloys; purification of liquid metals by chemisorption on particulate solids.

AMES LABORATORY
Chemistry Division -03- (Continued)

31. METALS FROM FLY ASH — $ 98,000 — 03-02
G. Burnet, M. J. Murtha

Recovery of iron oxide from power plant fly ash by magnetic separation and of alumina using calcination, selective chlorination and hydrochemical processing.

32. EMITTANCE PROPERTIES OF MATERIALS AT HIGH TEMPERATURES — $ 60,500 — 03-02
R. G. Bautista

Normal spectral emittance of liquid metal alloy systems; temperature measurements by optical pyrometry; spectral determinations on high temperature solar absorber candidate materials; quantitative characterization of surface roughness and its effect on the emittance properties of surfaces.

33. MASS TRANSFER AND TRANSPORT IN FLUIDS AND PARTICULATE SYSTEMS — $ 79,500 — 03-02
L. E. Burkhart

Particle and fluid motion in mass transfer systems by high speed photography and mathematical modeling; transport near interfaces, especially drops and bubbles; control of particle size distribution, growth and morphology in preparation of fine powders; reaction kinetics and mixing in multicomponent mass transfer systems involving chemical reactions.

34. HIGH TEMPERATURE CHEMISTRY — $164,500 — 03-03
H. F. Franzen, A. V. Hariharan

Structure and bonding in refractory compounds, particularly metal-rich transition metal chalcogenides and phosphides; high temperature stability and phase equilibria, X-ray photoelectron spectroscopy of refractory solids; high-temperature X-ray diffraction, mass spectrometry.

AMES LABORATORY
Chemistry Division -03- (Continued)

35. SURFACE CHEMISTRY AND CATALYSIS — $255,500 — 03-03
R. S. Hansen, B. C. Gerstein
K. G. Baikerikar, T. W. Orent

Heterogeneous catalysis by metals and semiconductors, clean surfaces, reactions associated with coal liquefaction and gasification, field emission microscopy, flash desorption spectriscopy, LEED and Auger spectroscopy; single crystal face catalysis; electrical double layer properties and their alteration by adsorption; mechanical and flow properties of interfaces; motion and electronic structure of adsorbed species by pulse and multiple pulse NMR.

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

Materials Science Division -01-
B. R. T. Frost - Phone: (FTS) 388-2221 or 312 739-2221
F. Nichols - Phone: (FTS) 388-2222 or 312 739-2222

36. ALLOY PROPERTIES — $356,000 — 01-01
F. Y. Fradin, A. T. Aldred,
D. J. Lam, B. W. Veal, Jr.

Electronic structure and its relationship to physical properties and bonding; emphasis on actinide compounds and actinide bonding in glasses; XPS studies of binding energies of ions U to Cf in oxide matrices; magnetic and nmr studies of 5f electron localization; EXAFS studies of the structure of transition metal ions in glasses.

37. PROPERTIES OF HIGH-TEMPERATURE MHD MATERIALS — $256,000 — 01-01
A. T. Aldred, D. J. Lam,
B. W. Veal, Jr., D. Karim

Studies of electronic structure of ceramic materials; electrical conductivity and magnetic susceptibility studies of $La_{1-x}Sr_xCrO_3$ ($X = 0.0, 0.02, 0.16$) from $T = 4$ to 2000 K and $P_{O2} = 1$ to 10^{-12} atm; XPS studies of valence bands and core-level structure of $LaCrO_3$, $LaFeO_3$, and $LaCoO_3$.

38. CATALYSIS AND SURFACE STUDIES — $159,000 — 01-01
M. B. Brodsky, S. D. Bader,
J. F. Blakely, T. Orent

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

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

39. SCATTERING STUDIES $576,000 01-01
M. H. Mueller, G. H. Lander

Magnetic, electronic and structural properties of actinide materials using neutron and x-ray scattering; internal rearrangements in UO_2 with extension to CeBi, UAs and to stabilized ZrO_2. Observation of conduction electron polarization directly in PuP and measurement of the anisotropy in the magnetic ground state. Inelastic neutron measurements on USb to measure exchange, anisotropy and crystal-field energies; search for phonon softening at the 43 K transition of αU; hydrogen position in storage metal hydrides of the $LaNi_5D_6$ type as well as MPd_3X_x where M is a transition metal, lanthanide or actinide; magnetic structure of the rare earth binary hydrides; pulsed inelastic neutron experiments on UO_2 and high-resolution powder application to perovskites and complex hydrides; design and possible uses for SANS at CP-5 and on a pulsed source.

40. PHYSICAL METALLURGY $259,000 01-01
M. B. Brodsky, A. J. Arko

Electronic structures of actinide metals, alloys, and compounds; low temperature specific heat measurements; electrical resistivity; magnetic susceptibility and Mossbauer effect of actinide alloys and compounds to study spin fluctuations and band magnetism; de Haas-van Alphen effect in actinide metals and compounds; scattering of electrons by lattice defects.

41. MECHANICAL PROPERTIES - EROSION AND WEAR $115,000 01-02
A. P. L. Turner, R. O. Scattergood, T. H. Kosel

Experimental investigation of the mechanisms of wear and erosion of metal and ceramic surfaces; examination of the damage layers formed by wear, utilizing scanning and transmission electron microscopy, for the purpose of determining the role of plasticity and the influence of microstructure on the wear process. Materials currently investigated: nickel, nickel alloys, MgO, alumina.

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

42. MECHANICAL PROPERTIES - PLASTICITY — $501,000 — 01-02
J. F. Kocks, R. A. Mulford, J. L. Routbort, R. O. Scattergood, A. P. L. Turner, H. Mecking, R. Schwarz

Theoretical and experimental research on the mechanical properties of metallic and ceramic solids: strengthening mechanisms (solutes, second phases, voids); strain hardening and recovery mechanisms (dynamic, static, cyclic); constitutive relations for plasticity, creep and fatigue of metals and ceramics, especially at elevated temperatures; structure characterization of deformed crystals by x-ray diffraction, electron microscopy, and internal friction; dislocation properties, kinetics, dynamics, statistics. Materials currently investigated: nickel alloys, stainless steel, copper, MgO.

43. SUPERCONDUCTIVITY — $307,000 — 01-03
F. Y. Fradin, G. S. Knapp, H. Chen

Studies of the effects of composition and degree of order on the strength of the electron-phonon interaction in binary and ternary compounds; nmr and Mossbauer effect studies of the interaction of spin polarized and superconducting electrons in Chevrel phases; EXAFS and nmr studies of the effects of defects on T_c in A-15 compounds; heat capacity and Mossbauer investigations of anharmonic behavior in high T_c compounds.

44. BASIC CERAMICS STUDIES — 01-03
N. L. Peterson, W. K. Chen, J. Faber, Jr., M. D. Rechtin, K. K. Kim

Ceramic materials fundamental research. Grain boundary and bulk diffusion of cations and point defect studies in metal oxides; transport properties in mixed oxide MHD candidate materials; ionic transport in the solid electrolyte sodium beta-alumina; allotropic phase transformations in perovskite oxides which are possible MHD materials and the effect of dopants on their properties; neutron scattering studies of order-disorder transitions in the superionic conductors of calcia and yttria stabilized zirconia; radiation damage microstructure of ceramic oxides subjected to ion bombardment at high temperature; and the effect of helium on the damage structure. (To be initiated in FY 1978).

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

45. METAL PHYSICS $827,000 01-03
R. W. Siegel, A. S. Berger,
W. K. Chen, E. S. Fisher,
M. J. Fluss, N. Q. Lam,
J. N. Mundy, S. J. Rothman,
D. G. Westlake, J. F. Miller,
R. P. Gupta, K. K. Kim,
L. C. Smedskjaer, S. W. Tam

The properties of atomic defects and defect clusters in solids; the atomic mechanisms of diffusion in solids; the nature and properties of metal-hydrogen systems; the elastic properties of solids; studies of point-defects and defect clusters in FCC and BCC-refractory metals using positron annihilation and electron microscopy techniques; vacancy-solute interactions using resistivity and electron microscopy; point-defect interactions with interfaces; tracer diffusion in Nb, W and intermetallic compounds; mechanisms of ionic transport in solid electrolytes; transport properties and cation diffusion in oxides; hydrogen solubility in Nb-Ta alloys; elastic and anelastic effects of interstitial impurities in transition metals.

46. DIFFUSION STUDIES $100,000 01-04
R. W. Siegel, N. Q. Lam,
S. J. Rothman

Effects of irradiation on tracer diffusion in W; theoretical studies of solute segregation during irradiation. (To be discontinued).

47. NEUTRON IRRADIATION $571,000 01-04
T. H. Blewitt, B. S. Brown,
M. A. Kirk, Jr., B. A. Loomis,
R. C. Birtcher, H. Lefakis

Point defect production, annihilation and clustering; radiation effects in superconductors; neutron sputtering; flux pinning of superconductors by defect clusters and voids; void nucleation in nickel and 316 stainless steel; replacement collision sequences; saturation effects and the recombination volume; void swelling in Nb and Nb-Zr alloys as a function of dose, temperature and oxygen content during simultaneous irradiation with 4 MeV Ni^+ and He^+ ions; radiation sources include the CP-5 low temperature facility and the 4 MeV Dynamitron.

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

48. CHARGED-PARTICLE IRRADIATION STUDIES — $620,000 — 01-04
K. L. Merkle, R. S. Averback, R. Benedek, R. L. Lyles, Jr., P. P. Pronko, W. B. Jager

Studies of defect structures and recrystallization in ion implanted solar materials; ion beam analysis of radiation-induced compositional changes and defect distributions. Correlation between 14 MeV neutron damage and heavy ion damage in metals. Properties of self-interstitials. Damage function studies by HVEM and ion irradiation. Studies of energy density effects in energetic cascades. TEM and HVEM of displacement cascades in binary alloys. Theory of sub-cascades formation. Interatomic potential calculations. Theoretical and experimental studies of properties of hydrogen and helium in metals. Effect of crystallinity on defect production. Application of channeling techniques to defect reactions. Defect cluster formation by HVEM. Major experimental facilities include 300 kV heavy ion accelerator, 14 MeV neutron source at LLL and high voltage electron microscope (being installed) with ion interface capability. In the future, a 2 MV ion accelerator and a low energy ion injector will be available for in-situ HVEM studies.

49. KINETIC STUDIES — $743,000 — 01-04
H. Wiedersich, F. V. Nolfi, Jr., P. R. Okamoto, D. I. Potter, M. D. Rechtin, A. Taylor, R. J. DiMelfi, L. E. Rehn, A. A. Sagüés

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; effect 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 formation during ion bombardment; damage structure produced during high-temperature ion bombardment of oxides; radiation sources include 300 keV heavy-ion accelerator, 4-MeV Dynamitron -- 2 MeV Van de Graaff Dual-ion-beam Facility, and high-voltage electron microscope (being installed).

ARGONNE NATIONAL LABORATORY
Solid State Science Division -02-
D. L. Price - Phone: (FTS) 388-3141 or 312 739-3141

50. NEUTRON SCATTERING STUDIES $1,190,000 02-01
T. Brun, G. Felcher,
R. Kleb, C. Pelizzari,
S. K. Sinha, R. Crawford,
J. D. Jorgensen, R. Maglic,
T. Postol, K. Skold

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. 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 liquids including He^3; dynamics of superconductors; crystal-field interactions and magnetic properties of transition metals and alloys and of rare-earth intermetallics; magnetic scattering in magnetically ordered systems; spin glasses and rare-earth magnetic form factors; high-pressure diffraction and compressibility measurements of metals, ionic crystals, ice and high-temperature ceramics.

ARGONNE NATIONAL LABORATORY
Solid State Science Division -02-
D. L. Price - Phone: (FTS) 388-3141 or 312 739-3141

51. PULSED NEUTRON SOURCE DEVELOPMENT — $0 — 02-01
J. M. Carpenter, R. K. Kleb

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. 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.

52. MATERIALS PREPARATION AND CHARACTERIZATION — $ 87,000 — 02-02
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 CsCl and Cu_3Au structures for magnetic studies, refractory oxides such as Y_2O_3 for studies of MHD electrode problems, and the alkali halides and cyanides.

53. DEFECTS IN NONMETALLIC SYSTEMS — $182,000 — 02-02
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. Areas of current interest include: the production and motion of vacancies and interstitials; excitation, tunneling recombination, and luminescence processes in heavy-metal centers in insulators; structure and reorientation dynamics of molecular-ion centers (F_2^-, Cl_2^-, $BrCl^-$) in alkali halides; ESR studies of F_2^- centers in alkali fluorides, thallium in alkali chlorides and manganese in calcite; and production and motion of interstitial molecular-ion species (FCl^-, $BrCl^-$ and ICl^-) in alkali halides.

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

54. LOW TEMPERATURE STUDIES $271,000 02-02
H. A. Kierstead,
P. Roach, R. Webb

Studies of properties of quantum liquids and solids at very low temperature. Current activities and areas of interest include: precision measurements of the thermodynamic properties of He^3, He^4, and He^3-He^4 mixtures near phase transitions; properties of superfluid phases of He^3; sound propagation and ion mobility in new He^3 phases; adiabatic cooling by nuclear demagnetization; development of SQUID NMR techniques for susceptibility measurements in the low millikelvin range; and static and dynamic susceptibility of He^3 phases.

55. SUPERCONDUCTIVITY STUDIES $320,000 02-02
K. Gray, C. Falco,
J. Hafstrom, C. Wu,
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 and electrical noise power measurements; dynamic behavior of flux structures; flux flow, flux pinning and the relaxation time for magnetic flux penetration; electrical and magnetic properties and superconductivity breakdown at very high transport currents; optical excitation of nonequilibrium states in superconductors; properties of magnetically-coupled superconducting films; Josephson weak links; the preparation of high T_c materials such as Nb_3Sn by high-rate sputtering; the development of high-temperature SQUIDS and superconducting switches.

56. CATALYSIS AND SURFACE STUDIES $242,000 02-02
D. O'Reilly, G. Crabtree,
C. Falco, G. Felcher,
R. Webb, L. Iton

The dynamics and properties of atoms and molecules adsorbed on surfaces as studies 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; studies of fluid statics and dynamics, and melting and condensation; inelastic electron tunneling through submonolayers of organic molecules; atomic-beam scattering from surfaces; and SQUID susceptibility and NMR measurements.

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

57. ELECTRONIC, MAGNETIC AND LATTICE PROPERTIES — $299,000 — 02-02
G. Crabtree, B. Dunlap, H. Kierstead, G. Shenoy, D. H. Dye

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 Au, Nb, Pt and Pt, the actinides and rare-earths and superconducting A15 compounds such as Nb_3Sb. Magnetic properties of metals, alloys and ocmpounds are studied with emphasis on local-moment vs. itinerant models of magnetism. Topics include Mossbauer effect measurements of hyperfine interactions, spin-lattice relaxation times and crystal-field effects in lanthanide and actinide-materials; studies of conduction-electron polarization in Chevrel-phase superconductors; the degree of localization 5f electrons in actinide Laves-phase intermetallics; investigation of ionic valence change and dislocation pinning in cold-worked materials; and studies of rare-earth hydride and hydrogen absorption in rare-earth and transition metals.

58. LIGHT SCATTERING AND ACOUSTICS — $ 74,000 — 02-02
P. R. Roach, J. 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.

59. SOLAR MATERIALS — $191,000 — 02-02
L. Guttman, J. A. 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; investigation of the random network model of amorphous materials; electronic structure of amorphous silicon; theory of bulk and surface optical properties; and sum-rule constraints on attainable optical properties.

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

60. REFRACTORY MATERIALS WITH MHD APPLICATIONS — $164,000 — 02-02
C. J. Delbecq, T. L. Gilbert, D. G. Hinks, J. J. Jackson, S. A. Marshall, W. Primak, S. Susman, P. H. Yuster, J. D. Jorgensen

Studies of refractory materials including the preparation and characterization of research samples of high-temperature oxides including Y_2O_3; optical ESR and ENDOR studies of electronic processes in the refractories Y_2O_3 and Al_2O_3 and yttrium aluminum garnet; theoretical studies of interatomic forces and local electronic structure in oxides; transport measurements at high temperatures.

61. SOLID STATE THEORY — $420,000 — 02-03
T. Arai, T. Gilbert, D. Koelling, F. Mueller, A. Rahman, J. Robinson, P. Vashishta, K. Lau, B. Yarlagadda

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 - non-metal transitions; surface phenomena including surface structure, physisorption, chemisorption and catalysis; electronic structure of perovskites; and theoretical studies of superionic conductors.

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

62. PARTICLE SOLID INTERACTIONS $280,000 02-04
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; distribution of defects; properties of divacancies and self-interstitial atom clusters and associated strain fields. Metals under study include platinum, rhodium, nickel, and indium. Studies of electromigration at high-temperatures in glasses and non-metal MHD electrodes; studies of surface radiation damage in insulators including work on lithium niobate, sapphire, spinel, lucalox, barium titinate, quartz, 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 in materials of CTR interest such as silicon nitride, zirconium oxides, silicon carbide, boron carbide and titanium boride.

ARGONNE NATIONAL LABORATORY
Chemistry Division -03-
P. R. Fields - Phone (FTS) 388-2666 or 312 739-2666

63. NEUTRON SCATTERING AND X-RAY DIFFRACTION STUDIES — $590,000 — 03-01
S. W. Peterson, M. Atoji, J. M. Williams, H. E. Flotow, A. H. Reis, E. G. Sherry, P. L. Johnson, A. J. Schultz

Synthesis, x-ray and neutron scattering studies of new platinum and iridium complexes which exhibit one-dimensional metallic conductivity; x-ray structure study of substituted ferrocene-TCNQ complexes; preparation and neutron diffraction studies of rare-earth metals and alloys and the tungsten bronzes; preparation and x-ray and EXAFS studies of graphite intercalation compounds; EXAFS studies of iron complexes in solution; x-ray and neutron studies of storage hydrides such as $LaNi_5D_6$; x-ray studies of organophosphate actinide extractants.

64. PHYSICAL AND SURFACE CHEMISTRY — $374,000 — 03-03
D. M. Gruen, R. L. McBeth, R. B. Wright, A. R. Krauss, M. H. Mendelsohn, J. K. Bates, M. B. Liu

Compound formation resulting from the bombardment and implantation of energetic reactive particles such as kilovolt H^+, D^+, O^+ and N^+; the effects of surface chemistry on the charge state, state of excitation, energy and angular distribution of sputtered surface atoms, molecules and ions; simultaneous energy analyzed secondary ion mass spectrometry and Auger analysis together with *in situ* XPS on clean and oxygen-covered Ti surfaces; quantitative measurements of ion sputtering yields; glancing angle energy-dispersive x-ray diffraction, TEM electron diffraction and SIMS profiling characterization of ion nitrided Ti and Zr; ion bombardment induced photon emission (SCANIIR) measurements on Ti and Be surfaces; matrix isolation spectroscopic studies of Au and Ag atoms in solid D_2 matrices and of MoN and ZrN molecules in Ar matrices; factors, such as configurational entropies, determining the stabilities of AB_5 hydrides; cell-volume stability correlations leading to the development of the new $AB_{5-x}Al_x$ ternary systems for hydrogen storage and chemical heat pump applications; vibrational and electronic spectroscopy of organic molecules in fused salt solutions; laser Raman profiling of ion-bombarded surfaces to study amorphization and annealing of displacement damage in surface and near surface regions.

ARGONNE NATIONAL LABORATORY
Chemistry Division -03- (Continued)

65. LOW TEMPERATURE CALORIMETRY $158,000 03-03
D. W. Osborne, H. E. Flotow

Heat capacity measurements and determination of entropies, enthalpies and Gibbs energies from 0.1 to 350 K for use in thermodynamic calculations at higher temperatures; emphasis is placed on inorganic compounds of importance in nuclear energy systems and in non-nuclear energy systems; among the compounds currently being studied are: plutonium oxides, nitrides and carbides made from the longer-lived plutonium isotope ^{242}Pu; uranium oxides, sulfides and selenides; sodium-uranium-oxygen compounds; U_3Si (a possible fuel for a new reactor); compounds of high-yield fission products (e.g., Cs, Ba and Mo) with uranium and chromium; lanthanide trifluorides; $KAlO_2$, $CsAlO_2$, $CsNO_3$, Cs_2CO_3 and other compounds that may be involved in the coal-fired magnetohydrodynamic process; lithium-aluminum alloys and Li_2S for the battery program; compounds involved in cycles for the thermochemical decomposition of water.

66. HIGH-TEMPERATURE CHEMISTRY $408,000 03-03
R. J. Thorn, R. J. Ackermann,
J. R. McCreary, E. G. Rauh,
G. E. Murch, W. Y. Howng,
R. Sheldon, 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 and altered valent or aliovalent cations in non-stoichiometric 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 to 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 non-stoichiometric phases; studies of molecular ions present in thermal excursions in reactors; evaluation of thermochemical systematics and data of lanthanide and actinide phases; materials studied: oxides, carbides, sulfides, fluorides of uranium, thorium, plutonium, lanthanides, zirconium, silicon and aluminum, and intermetallics of uranium, thorium, tungsten, tantalum and rhenium.

ARGONNE NATIONAL LABORATORY
Chemical Engineering Division -03-
L. Burris - Phone: (FTS) 388-2594 or 312 739-2594
F. Cafasso - Phone: (FTS) 388-3672 or 312 739-3672

67. LIQUID METALS CHEMISTRY $185,000 03-02
V. A. Maroni, E. Veleckis,
W. Calaway, R. M. Yonco

Thermodynamic and transport properties of liquid alkali metals and their solutions; phase diagrams and solution thermodynamics of LiT_2, Li-Al-H_2, Li-Pb-H, Li-Si-H, and Li-K-H systems by tensimetric methods; pressure composition isotherms for LiH and LiD in liquid lithium below the monotectic; Li-H, -D, -T isotope effects; Li-Li_3N, Li-LiO_2, and Li-Li_2C_2; analysis of stable carbon bearing species in molten lithium; phase diagrams; 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 mechanism of refractory metals and alloys in liquid lithium.

68. MOLTEN SALT CHEMISTRY $180,000 03-02
M. Blander, G. Papatheodorou,
M. Saboungi

Calculation of phase diagrams and other thermodynamic properties of molten salts using fundamental solution theories; solubilities of oxides and sulfides in molten salts; conformal ionic solution theory; thermodynamic and spectroscopic properties of salt vapors; identification of high temperature associated vapor species formed between acidic salts as $AlCl_3$, and $ZnCl_2$ and other salts; spectra of $CoBr_2 \cdot n\ AlBr_3$, $PdCl_2 \cdot n\ InCl_3$, $CuCl_2 \cdot n\ AlCl_3$; spectra of carbonium ions in acidic molten salts, stabilization of carbonium ions, catalytic activity of $ZnCl_2$ and $AlCl_3$: vapor-transport measurements, chemical separations using vapor-transport.

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

69. CHEMISTRY OF MATERIALS — $330,000 — 03-02
R. Kumar, B. Holt, B. Hubble,
H. R. Isaacson, S. Johnson

Chemistry of sulfate and nitrate airborne particles and their formation mechanisms; methodology for aerosol characterization; size, time, and spatial variations in the chemistry of airborne particles; IR method for quantitative measurement of acidic sulfate; GC-FID method for atmospheric poly-nuclear aromatics; attenuated total reflectance spectroscopy; stable isotope-ratio method for study of mechanisms of SO_2 oxidation in atmosphere; kinetics of sulfur fixation by half-calcined dolomite and of the regeneration of the active material from sulfated calcine, mechanism of reactions, micro-morphology studies, thermogravimetric analysis, differential thermal analysis, X-ray diffraction and SEM studies.

70. CALORIMETRIC STUDIES OF ENERGY RELATED MATERIALS — $125,000 — 03-02
C. E. Johnson, W. N. Hubbard,
G. K. Johnson, K. Kim

Experimental thermodynamic properties of organic and inorganic materials; interpretation and prediction of materials properties such as enthalpies of formation and bonding energies; standard enthalpies of formation (ΔH_f°-H_{298}); oxygen and fluorine bomb calorimetry, hypergolic reaction calorimetry, titration calorimetry, flow calorimetry, drop calorimetry to 200 K; enthalpies of formation of (1) building block molecules of coal, e.g., xanthone, benzofuran, benzopyrene, chrysene, and (2) gadolinium, dysprosium, and holmium trifluorides; calorimetry studies on Cs_2CrO_4, Cs_3CrO_4, Cs_4CrO_4, UN, U_2N_3, ThN, Cs_2ThO_3.

71. PHYSICAL CHEMISTRY OF ELECTRO-CHEMICAL ENERGY STORAGE — $185,000 — 03-02
Z. Nagy, C. Melendres,
M. Blander, M. Saboungi

Electrochemical studies of processes occurring at cell electrodes and in electrolytes, lithium-aluminum/LiCl-KCl/metal sulfide system studies; electrode reaction kinetics and mechanisms; charge transfer processes; metal deposition/dissolution reactions; electronic and ionic conductivity; electromotive force measurements; lithium-aluminum, lithium-lead, lithium-aluminum-magnesium; solution thermodynamics, chemical activities; phase diagram of lithium-aluminum, lithium-magnesium, magnesium-aluminum, lithium-calcium, calcium-magnesium; prediction of ternary phase diagrams from subsidiary binaries; pseudopotential theory; thermodynamic properties of ternary alloys.

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

72. HEAT TRANSFER MATERIALS AND METASTABLE FLUIDS — $115,000 — 03-02
M. Blander, L. Curtiss

Studies on materials which exhibit strong or unusual bonding in the vapor and, hence, are potentially useful as heat transfer fluids; nature of vapor species; equilibrium constants; relative bond strengths; thermal conductivities; methanol, trifluoroethanol and pyridine; hydrogen bonding; P-V-T properties of stable and metastable fluids and testing of equations of state; contact vapor explosion mechanisms; nucleation theory; molecular dynamics, calculations; heterogeneous nucleation of water.

73. SURFACE AND MORPHOLOGICAL STUDIES ON ELECTROCHEMICAL SYSTEMS — $ 50,000 — 03-02
F. A. Cafasso, S. Siegel, C. Melendres

Surface, structural, and morphological investigations of selected electrode systems; electrocatalysis; electrode degradation, electrode wetting and dewetting phenomena; dendrite growth processes; LiAl and LiAlMg electrodes; Mossbauer spectroscopy, X-ray diffraction, scanning electron microscopy.

74. METALLURGICAL PROCESS SCIENCE AND ENERGY CONSERVATION — $110,000 — 03-02
M. Blander, M. Saboungi, Z. Nagy

Studies of fundamental chemistry of energy saving environmentally acceptable metallurgical processes; chemistry of electrowinning of aluminum from cryolite and from chloride melts, complexing of Al^{+3} and $O^{=}$ ions in chloride melts, phase diagrams of cryolite containing systems, electromotive force measurements of complexing, solubilities of sulfides in molten salts, direct electrolysis of sulfides.

BROOKHAVEN NATIONAL LABORATORY
Upton, Long Island, New York 11973

Corrosion Group -01-
D. H. Gurinsky - Phone: (FTS) 664-3504 or 516 345-3504
J. R. Weeks - Phone: (FTS) 664-2617 or 516 345-2617

75. INTERGRANULAR STRESS CORROSION OF IRON AND NICKEL BASE ALLOYS — $130,000 — 01-02
J. R. Weeks, Brijesh Vyas
M. W. Kendig

Electrochemistry of surfaces of iron and nickel base alloys under stress as revealed by scanning reference electrode and a-c polarization techniques. Determination of sensitization of stainless steel using these techniques and measurements of grain boundary segregation of the consequences of these alloys using energy dispersive x-ray analysis attached to a transmission electron microscope.

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

76. RELATIONSHIP BETWEEN PROPERTIES AND STRUCTURES — $800,000 — 01-03
R. Caton, D. Dew-Hughes,
D. H. Gurinsky, O. Kammerer,
K. Lee, C. Pande, M. Pick,
M. Suenaga, D. Welch
A. Arbel

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 A-15 superconductor formation in solid state diffusion process: Mechanical deformation process in A-15 superconductors: Physical properties of metal hydrides, FeTi, V_2Sr, V_2Hf: Hydrogen embrittlement, Fe whiskers, deformed Ni.

77. RADIATION DAMAGE — $180,000 — 01-04
C. L. Snead, S. Moehlecke

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 A-15 superconductors; defect and microstructure changes in irradiated materials; enhanced diffusion applied to A-15 superconductors by solid state process; application of positron annihilation to defect studies: voids and gases in metals.

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

78. NEUTRON SCATTERING - MAGNETIC SYSTEMS $505,000 02-01
G. Shirane, J. D. Axe,
L. Passell, S. M. Shapiro,
J. A. Tarvin, W. C. Thomlinson

Neutron scattering studies of the structure and dynamics of magnetic materials: spin dynamics of substitutionally disordered, low-dimensional antiferromagnets; spin dynamics of amorphous ferromagnets; excitations of itinerant ferromagnets; magnetic ordering in mixed superconducting-ferromagnetic systems; spin dynamics of mixed valence systems.

79. NEUTRON SCATTERING - PHASE TRANSITIONS $545,000 02-01
G. Shirane, J. D. Axe,
S. M. Shapiro, J. Eckert,
W. D. Ellenson

Neutron scattering studies of structural phase transitions and their dynamics; dynamics of incommensurate phase transitions; critical scattering in ferroelectric transitions; soft phonon modes in solids.

80. NEUTRON SCATTERING - ELEMENTARY EXCITATIONS IN SOLIDS $485,000 02-01
G. Shirane, J. D. Axe,
L. Passell, S. M. Shapiro,
J. Eckert, W. D. Ellenson,
W. C. Thomlinson

Neutron spectroscopy of low-lying excited states in solids; lattice dynamics of high pressure phases of solid ^4He; lattice dynamics of solid N_2 and CO_2; lattice dynamics of intercalated graphite.

81. NEUTRON SCATTERING - PARTIALLY ORDERED SYSTEMS $490,000 02-01
L. Passell, S. M. Shapiro,
J. Eckert, W. D. Ellenson,
J. A. Tarvin, W. C. Thomlinson

Neutron scattering studies of short-range order and excitations in partially ordered systems: structure and dynamics of ethylene monolayers adsorbed on graphite, dynamics of solid electrolytes; dynamics of thin superfluid ^4He films adsorbed on graphite.

BROOKHAVEN NATIONAL LABORATORY
Physics Department -02- (Continued)

82. EXPERIMENTAL RESEARCH - SUPERCONDUCTIVITY $355,000 02-02
M. Strongin, A. Ghosh,
H. Lutz, D. L. Miller

Superconductivity in A-15 films; studies of normal state resistivity of Nb_3Ge and Nb_3Sn films; studies of effects of α-particle and electron irradiation on the transition temperature and density of states; codeposition of elements to study metastable phases in alloy films; studies of hydrogen in amorphous silicon films.

83. EXPERIMENTAL RESEARCH - SURFACE STUDIES $110,000 02-02
M. Strongin, J. Strozier,
M. Yu

Use of ac pulsing techniques under ultra-high vacuum conditions to study chemical reactions such as the oxidation of CO on the surfaces of single crystal and polycrystalline Group VIII metals (Pt, Pd, Rh, Ru, etc.), and transition metals oxides. Understanding and development of secondary ion mass spectroscopy for chemisorption studies; correlation with chemisorption bonds and surface phases. Interaction of low energy ions with surfaces.

84. EXPERIMENTAL RESEARCH - SPECTROSCOPY OF SOLIDS $225,000 02-02
B. C. Frazer, H. Engstrom,
J. M. Hastings

Studies of structural, dynamic, and electronic properties of solids by x-ray, neutron, and light scattering. Preconstruction R&D on National Synchrotron Light Source (NSLS). Defect-induced Raman spectra from $NaClO_3$ and Al_2O_3. Neutron scattering from hydrogen-reduced $SrTiO_3$ in relation to "central peak" problem and defect-induced modifications of low lying lattice modes in superconducting range of carrier concentrations.

BROOKHAVEN NATIONAL LABORATORY
Physics Department -02- (Continued)

85. THEORETICAL RESEARCH — $460,000 — 02-03
V. J. Emery, M. Blume, G. J. Dienes, J. F. Herbst, S. Krinsky, R. H. Swendsen, R. E. Watson, D. O. Welch, S. Aubry

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; properties of superionic conductors; radiation induced conductivity; molecular dynamical calculations of equations of state and shock waves; studies of valence electron distributions in crystals.

86. PARTICLE-SOLID INTERACTIONS - RADIATION EFFECTS RESEARCH — $520,000 — 02-04
A. N. Goland, P. W. Levy, K. G. Lynn, K. J. Swyler

Studies of neutron- and electron-irradiated metals and alloys employing positron-annihilation lifetime and Doppler-broadening measurements; simultaneous optical absorption and luminescence measurements during electron irradiation of ceramics, glasses and alkali halides; radiation-damage analysis of fusion and fission reactor materials studies.

87. PARTICLE-SOLID INTERACTIONS - PROPERTIES OF REAL SOLIDS — $495,000 — 02-04
A. N. Goland, P. W. Levy, J. E. Dickman, H. Engstrom, K. G. Lynn

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; channeling of protons in very-thin single crystals; applications of μ+SR to defect problems in solids; geophysics of mineral thermoluminescence.

BROOKHAVEN NATIONAL LABORATORY
Physics Department -02- (Continued)

88. ADVANCED MATERIALS SYNTHESIS AND CHARACTERIZATION — $130,000 — 02-04
D. E. Cox, B. C. Frazer, C. Khattak

High-temperature oxides and high T_c superconductors; preparation of the simple oxides Al_2O_3 and Y_2O_3 and various perovskite oxides for MHD systems; electrical conductivity, x-ray and neutron diffraction studies of pure and doped crystals of $LaCrO_3$ system, $BaCeO_3$, $SrCeO_3$, $BaZrO_3$, $BaCoWO_6$, and Ba_2MnWO_6; structural studies of defect fluorites based on the ZrO_2 and CeO_2 systems; x-ray studies of vapor deposited Nb-Ge alloys and synthesis of Nb_3Sn single crystals.

89. PARTICLE-SOLID INTERACTIONS - ALTERATION AND ANALYSIS OF SOLIDS BY ION BEAMS — $60,000 — 02-04
A. N. Goland, J. S. Rosner, M. Strongin

Alloy formation and modification by ion implantation, high-resolution Rutherford backscattering for analysis, ion-induced lattice damage, channeling phenomena, studies of defect structure of A-15 superconductors.

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Idaho Falls, Idaho 83401

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90.	WELDING RESEARCH J. F. Key	$0	01-05

Modelling of heat-source/molten-pool interactions; post weld embrittling mechanisms; age hardenable nickel base alloys; grain boundary characterization; influence of trace elements and oxygen in the embrittlement process (to be initiated in FY 1978).

91.	GEOTHERMAL SCALING AND CORROSION RESEARCH D. E. Michels	$120,000	03-03

Chemical mechanisms in scaling and corrosion; tests in simulated geothermal brines; crystal growth from solutions on selected substrates; rotated-disc electrode apparatus used to establish preselected hydrodynamic conditions on substrates; deposition of calcite on metallic substrates; corrosion of iron alloys in solutions containing silica and ionic salts; deposition of silica on Fe; effects of stress and trace elements; x-ray diffraction, LEED, AES, and acoustic emission.

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Urbana, Illinois 61801

Materials Research Laboratory -02-
R. J. Maurer - Phone: 217 333-1370
C. P. Flynn - Phone: 217 333-0116

92. LOCALIZED CORROSION OF PASSIVE METALS — $47,000 — 01-01
R. C. Alkire

Corrosion of metal surfaces during fluid flow. Influence of surface impurities. Erosion by particle impaction and cavitation. Mechanism of stress corrosion cracking.

93. DYNAMIC STRUCTURE OF SUPERCRITICAL DENSE WATER AND AQUEOUS ELECTROLYTE SOLUTIONS — $101,000 — 01-01
J. Jonas

Dynamic structure of water and electrolytes under extreme conditions of temperature and pressure. Use of high pressure supercritical steam for isotope enrichment. Structure of disordered organic solids and polymers.

94. DEFORMATION IN REINFORCED METALS — $27,000 — 01-02
M. Metzger

Development of realistic models, using the system Ni_3Al-Ni_3Nb, for the prediction of the mechanical behavior of metal-matrix composites.

95. APPLICATIONS OF ELECTRON MICROSCOPY IN MATERIALS SCIENCE — $48,000 — 01-02
H. L. Fraser

Development and application of analytical and transmission electron microscopy techniques to determine morphology, microstructure, crystal and electronic structure and microchemistry of metallic alloys. Applications include the omega phase transformation in Zr-Nb alloys, iodine embrittlement in Zr alloys, the alpha-beta interface in Ti-Al-V alloys, precipitation in Nb-Ti-C alloys.

96. HYDROGEN BEHAVIOR IN BCC METALS — $135,000 — 01-02
H. K. Birnbaum

Mobility and quantum diffusion mechanisms of hydrogen, deuterium, tritium and helium in niobium, tantalum, vanadium and palladium. Properties and phase transitions of the Group Vb metal hydrides.

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

97. INTERSTITIAL SOLID SOLUTIONS $50,000 01-02
C. J. Altstetter

Effect of dissolved oxygen on the mechanical properties of niobium, tantalum, vanadium and their alloys. Effect of solutes, precipitate phases, polycrystallinity, and surface roughness on ion beam sputtering of niobium.

98. PRECIPITATION IN REFRACTORY METAL ALLOYS $37,000 01-02
C. A. Wert

The formation and effect on mechanical properties of carbide, oxide and hydride precipitates in V-Ti-C alloys, V, Nb, and Ta. Determination of the reduction paths in the extraction of W from WO_3.

99. THE MECHANISM OF STRESS-CORROSION CRACKING PROPAGATION STUDIES $79,000 01-02
E. N. Pugh

Determination of the mechanisms of stress corrosion cracking and hydrogen embrittlement of engineering materials. Materials investigated include Mg-Aℓ alloys, zircalloy, Admiralty metal.

100. PHYSICAL AND CATALYTIC PROPERTIES OF CATALYSTS $49,000 01-03
G. P. Wirtz

Investigation of the La-Co-O system as a model for rare earth perovskite catalysts. Defect structure and oxygen mobility in $LaCoO_3$ are related to catalytic activity. Development of thallic oxide films for heat mirrors of solar energy collectors.

101. NUCLEAR MAGNETIC RESONANCE STUDIES OF METALS AND POLYMERS $50,000 01-03
T. J. Rowland

Nuclear magnetic resonance investigation of crosslinking in polymers and of the structure of organic charge transfer coumpounds.

102. DIELECTRIC SOLIDS $43,000 01-03
D. A. Payne

The synthesis of single and polycrystalline piezo, pyro, and ferroelectric ceramics by hydrothermal, flux, and liquid phase sintering techniques. Characterization of dielectric properties. Growth and characterization of diphasic mixtures of $BaTiO_3$ and $Pb_5Ge_3O_{11}$ for low loss, high dielectric constant applications.

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

103. LOW TEMPERATURE STUDIES OF DEFECTS IN SOLIDS — $82,000 — 02-02
A. C. Anderson

Low temperature investigation of the effect of lattice defects and interfaces on thermal transport; of disordered superionic materials particularly beta alumina; of interstitial hydrogen in niobium. Development of low temperature thermometers.

104. RESPONSE OF SOLIDS TO ELECTROMAGNETIC RADIATION — $57,000 — 02-02
J. Dow

Optical properties of III-V semiconductor compound laser materials. Effect of synchrotron radiation on metals. Nature of intercalation in transition metal dichalcogenides.

105. USE OF VERY HIGH PRESSURE TO INVESTIGATE THE STRUCTURE OF MATTER — $135,000 — 02-02
H. G. Drickamer

Use of very high pressure techniques to investigate the mechanism of energy transfer in inorganic solid phosphors and liquids; to investigate organic photochemistry, photoconductivity and photochemical reactivity; to study the interaction of solutes with polymers.

106. ANHARMONIC EFFECT IN SOLIDS — $85,000 — 02-02
A. V. Granato

Ultrasonic investigation of the structure of interstials in radiation damaged metals; of the strength of metals; of non-linear elastic effects that determine the thermal properties of solids.

107. IMPURITIES IN SUPERCONDUCTORS — $73,000 — 02-02
D. M. Ginsberg

The effect of hydrogen on the properties of superconductors. The interaction of magnetic impurities with the electrons of superconductors.

108. DEFECT PROPERTIES OF SOLIDS — $96,000 — 02-02
D. Lazarus

Atomic mobility in the anomalous bcc transition metals like Ti and its alloys and in the superionic conductors like AgI and $RbAg_4I_5$.

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

109. PROPERTIES OF NOBLE GAS CRYSTALS $74,000 02-02
R. O. Simmons

The structure of thermal defects in helium crystals. Quantum effects in diffusion in crystals. Phase transformations in simple molecular crystals. Phonon-phonon interactions in insulating crystals with large lattice anharmonicities.

110. NUCLEAR MAGNETIC RESONANCE IN SOLIDS $115,00 02-02
C. P. Slichter

Nuclear magnetic resonance investigations of magnetic atoms in nonmagnetic metals (Kondo effect); of layered compounds and charge density waves; of platinum-silica reforming hydrocarbon catalysts; of deep traps in semiconducting photovoltaic solar energy convertors.

111. PHYSICS OF REFRACTORY MATERIALS $127,000 02-02
W. S. Williams

The physical properties of the transition metal carbides with emphasis on hardness, catalytic properties, and possible use as photothermal solar energy convertors.

112. RADIATION DAMAGE IN SOLIDS $130,000 02-04
J. S. Koehler

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

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Berkeley, California 94720

Materials and Molecular Research Division
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113. MICROSTRUCTURE, PROPERTIES AND ALLOY DESIGN - ELECTRON DIFFRACTION AND MICROSCOPY — $330,000 — 01-01
G. Thomas

Relationships between microstructure and properties; control of properties through characterization and control of structure; application of principles of strengthening and phase transformations to alloy design for mechanical and magnetic property improvements - energy conservation; systems under investigation include ferrous alloys, steels, alloys undergoing spinodal and ordering transformations, and ceramics. Quantitative analyses of structure by high resolution electron microscopy and diffraction and high voltage electron microscopy.

114. 1.5 MeV ELECTRON MICROSCOPE — $30,000 — 01-01
K. Westmacott

Point defect clusters: the object of this research is to understand in detail the nature of point defect clusters and the factors that affect the formation of various types of secondary defect. HVEM equipment plans: the 650 kV microscope will be modified to adopt a side-entry specimen stage and an environmental chamber for new research programs. Future programs involve the planning and management of the new 1.5 MeV microscope (installation expected 1978/79).

115. POWDER METALLURGY — $140,000 — 01-01
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)

116. THEORETICAL PROBLEMS IN ALLOY DESIGN — $255,000 — 01-02
J. W. Morris, Jr.

Mechanical properties of alloys: quantitative characterization of microstructure. Use of analytic, computer simulation, and experimental techniques. Alloy design: design of new engineering alloys to meet advanced requirements in the energy area. Current research: (1) ferritic Fe-Ni alloys combining high strength and high toughness at liquid helium temperature for use in superconducting devices; (2) tough ferritic Fe-Mn alloys for use as nitrogen temperatures, and (3) austenitic alloys which can be thermally processed to high strength and toughness for use in retaining rings in large electrical generators.

117. FUNDAMENTALS OF ALLOY DESIGN — $510,000 — 01-02
E. Parker, V. Zackay

Basic research on solid state transformation reactions: morphology of coherent precipitates for strengthening non-ferrous metals; bainitic transformation kinetics. Microstructure and mechanical properties: effect of silicon on stress corrosion cracking of high-strength steel; influence of retained austenite on tempered martensite embrittlement in ultra-high strength steels; influence of TRIP phenomena on the toughness of heat treatable alloy steels. New alloy developments: synergistic effects of alloying elements on tempering reactions involving austenite decomposition; new nickel-free stainless steels; mechanical properties of electroslag refined 300-M steel. Erosion-corrosion investigations; effect of microstructure on solid particle erosion resistance of ductile alloys. Continuum mechanics projects: effects of microstructure and load ratio on fatigue crack propagation in ultra-high strength steel; comparison of toughness evaluation of high-strength steel; comparison of toughness evaluation of high-strength steel by Charpy and K_{IC} tests; electrical potential technique for crack initiation measurement in fracture toughness testing.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

118.	RELATIONS BETWEEN DISLOCATIONS, POINT DEFECTS AND PROPERTIES OF METALS J. Washburn	$215,000	01-02

Elevated temperature radiation damage effects in metals and alloys: fundamental understanding of the factors that affect radiation induced swelling and creep based on high voltage electron microscope observations of dislocation climb and glide motion. Ion implantation effects in silicon: point defect clustering, dopant element precipitation, mechanisms of mass transport and effects of defects on electrical properties. Improved materials for solar energy utilization: the effects of substitution of Zn for some of the Cd in the conventional Cds-Cu_x-S solar cell. Structure and recrystallization behavior of "amorphous" silicon layers. Investigation of relation between structure and spectral selectivity of "black chrome" solar absorber coatings.

119.	ELEVATED TEMPERATURE EROSION-CORROSION BEHAVIOR OF MATERIALS A. Levy	$300,000	01-02

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

120.	SUPERCONDUCTIVITY EFFECTS - HIGH FIELD SUPERCONDUCTIVITY M. Pickus	$190,000	01-03

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 nad preferential precipitation sites such as regions of high strain energy.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

121. MICROSTRUCTURE AND MECHANICAL BEHAVIOR OF CERAMIC MATERIALS: GLASS AND CERAMIC-METAL SYSTEMS — $163,000 — 01-03
J. A. Pask

Kinetics and mechanisms of solid state reactions, nucleation and growth phenomena, sintering, and distribution of phases in a multiphase system. Mechanisms of corrosion attack on single crystal and polycrystalline ceramic materials. Structural, thermodynamic, and electrochemical studies of glass-metal and ceramic-metal systems; wetting, bonding, and nature of the interface; thermodynamics and kinetics of chemical reactions at such interfaces; kinetics and mechanisms of dissolution and diffusion in glasses.

122. HIGH TEMPERATURE REACTIONS — $215,000 — 01-03
A. Searcy

Torsion effusion and torsion-Langmuir measurements on the rate of decomposition of dolomite ($MgCO_3.CaCO_3$) in vacuo. Factors responsible for the formation of a metastable, reactive form of CaO. Rate and mechanisms of gas transport through pores of the metastable CaO. Gaseous and solid products formed by decomposing $Al_2(SO_4)_3$ in a mass spectrometer. Solution thermodynamics of solid $CaCO_3$. Theoretical studies on the kinetics of dissociative vaporization and of surface thermodynamics.

123. RELATION OF MICROSTRUCTURE TO PROPERTIES IN CERAMICS — $182,000 — 01-03
R. Fulrath *

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. Piezoelectric and ferroelectric properties in ceramic materials. Thick film conducting systems ceramic substrates; bonding, microstructure in the metallic phase, reduced precious metal contents.

* Deceased

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

124. STRUCTURE AND ELECTRICAL PROPERTIES OF COMPOSITE MATERIALS — $100,000 — 01-03
R. Bragg

Carbon Materials: Structure, electrical and mechanical properties of Glassy Carbon in the range of 1000°C - 3000°C. Use of wide range X-ray diffraction and small angle X-ray scattering techniques, Hall Effect and magnetoresistance - in the range 4.2 - 300°K in magnetic fields up to 50 KOe. Interpretation of the non-graphitizing nature of hard carbons. Composites: Aligned two-phase microstructures obtained by directional solidification of eutectic alloys. Effect of morphology on properties of composites; theory to predict properties, electrical measurements used as a predictor.

125. FAR INFRARED SPECTROSCOPY — $157,000 — 02-02
P. L. Richards

Improved infrared techniques are being used to do experiments in areas of fundamental and applied infrared physics where their impact is expected to be large. Programs in progress include measurements of the infrared radiation left over from the creation of the universe, measurements of the radiation from dust clouds in our galaxy, measurements of the infrared spectra of impurities in semiconductors, and measurements of the absorption spectra of the surface layers of liquids and solids.

126. EXPERIMENTAL SOLID STATE PHYSICS AND QUANTUM ELECTRONICS — $195,000 — 02-02
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 if interest, such as laser isotope separation, photochemistry, and surface phenomena.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

127. EXCITED QUANTUM FLUIDS IN SOLIDS — $110,000 — 02-02
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.

128. SUPERCONDUCTIVITY, SUPERCONDUCTING DEVICES, AND 1/f NOISE — $188,000 — 02-02
J. Clarke

Superconducting Quantum Interference Devices (SQUIDS) for measuring small fluctuations in magnetic fields and magnetic field gradients are being developed. The goal is to construct highly reliable and easily operated devices using an integrated thin-film technology in which the SQUID and the superconducting pick-up loops that couple magnetic flux to it are deposited on a single substrate. Detailed calculations of the intrinsic noise of these devices are being used to optimize the various design parameters. The use of these magnetometers for geophysical exploration is under investigation. A superconducting bolometer, the most sensitive available for broadband measurements in the far infrared, is also being developed. The microscopic origins of low frequency flicker noise in metal films are under investigation. The properties of non-equilibrium superconductors are being studied, for example, the enhancement of the energy gap and transition temperature by microwaves.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

129. THEORETICAL SOLID STATE PHYSICS $50,000 02-03
M. Cohen

Theoretical analyses aided by computer calculations are used to explain existing experimental phenomena and to predict new properties of materials such as: surface states on clean semiconductors; electrons at steps; vacancies and adsorbates on semiconductors; microscopic theory of metal-semiconductor interfaces (Schottky barriers); electronic structure of transition metal surfaces; bulk electronic and optical properties of solids, and superconducting transition temperatures for arbitrary electron-lattice coupling.

130. LOW TEMPERATURE PROPERTIES OF MATERIALS $105,000 03-01
N. E. Phillips

General objectives: obtain low-temperature heat-capacity data that contribute to an understanding of the relations between atomic properties and the macroscopic properties of materials. The materials investigated include normal and superconducting metals, super-fluids, dielectric solids, and magnetic materials. Heat capacity measurements are confined to temperatures below 25K because usually only in that region can various contributions be reliably separated. Establishment of a temperature scale for the region from 0.06 to 25K 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.

131. HIGH PRESSURE CHEMISTRY $40,000 03-01
G. Jura

Objectives: Determination of the heat capacities of metals and alloys as a function of temperature and pressure; determination of heat conductivities of non-metals 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.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

132. ELECTROCHEMICAL PROCESSES $105,000 03-01
C. W. Tobias

This program is designed to advance the scientific foundations of electrochemical engineering, and to widen the range of useful applications of electrochemical transformations. Mass and charge transport in cell processes; combined influences of electrode geometry, surface potential, and ionic transport; distribution of current on electrode macroprofiles in high-rate anodic dissolution and deposition of metals. Non-aqueous ionizing media for potential use at ambient temperatures in electrosynthesis and galvanic cell processes; thermodynamic and kinetic properties of electrode reactions which are not feasible in aqueous media. Electrolytic gas evolution; surface and electrolyte properties, hydrodynamic conditions, supersaturation, bubble nucleation, coalescence, and separation.

133. HIGH TEMPERATURE THERMODYNAMICS $80,000 03-03
L. Brewer

Characterization of the high-temperature chemical behavior of materials, particularly refractory ceramic materials, metals and gases. The high temperature thermodynamic properties are being determined through use of solid-electrochemical cells, solid-gas equilibria, and by X-ray 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.

134. CHEMISTRY AND MATERIALS PROBLEMS IN ENERGY PRODUCTION TECHNOLOGIES $125,000 03-03
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; molecular beam studies of gas-solid reactions, and radiation-enhanced stress corrosion cracking of metals.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

135. CRYSTALLIZATION KINETICS $50,000 03-03
L. F. Donaghey

Development of solid state materials processing methods, determination of models for prediction and control. Relationship of morphological, physical, electronic and structure-sensitive properties to processing conditions. Major processes: chemical vapor deposition, reactive sputter deposition, and solidification. Thermodynamic properties of solid state materials and their alloys, kinetic properties of processing methods, physical, structural and electronic properties.

136. ELECTROCHEMICAL PHASE BOUNDARIES $130,000 03-03
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.

137. SOLID STATE AND SURFACE REACTION STUDIES $230,000 03-03
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.

138. NUCLEAR MAGNETIC RESONANCE $105,000 03-03
A. Pines

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

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139. HOT CORROSION STUDIES RELATED TO FOSSIL FUELS — $170,000 — 01-01
D. W. Short, O. Krikorian

Mechanisms and kinetics of hot corrosion; quantitative model to relate the susceptibility of nickel and iron base alloys to corrosive media at elevated temperatures (800 to 1000°C); early stages of corrosion; kinetics studied by weight change and scale growth; salt-substrate interactions; molten salt electrochemical reactions; effects of oxide additions to a given salt; thermodynamic property measurements on the Cr-S system.

140. RAPIDLY QUENCHED AMORPHOUS MATERIALS RESEARCH — $ 60,000 — 01-03
C. Cline, R. Hopper

Selection, preparation and preliminary screening of amorphous alloys based on W, Be and B; 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.

141. LOW INDEX OPTICAL MATERIALS RESEARCH — $200,000 — 02-02
M. Weber, C. Cline

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.

142. OPTICALLY-INDUCED DAMAGE IN TRANSPARENT DIELECTRIC MATERIALS — $ 60,000 — 02-02
D. Milam, M. Weber

Laser damage in transparent dielectric materials as a function of pulse duration at 1064 nm, 532 nm, 355 nm, and 266 nm; materials include optical glasses, alkali halides and fluorides, and thin films; studies of electron avalanche, multiphoton absorption, bulk absorption and nonlinear absorption.

LAWRENCE LIVERMORE LABORATORY (Continued)

143. THIN FILM MATERIALS STUDIES FOR LASER OPTICAL COATINGS — $200,000 — 02-02
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.

144. D_2-DT-T_2 PHASE DIAGRAM — $120,000 — 03-02
J. Pyper, C. Souers

To determine the phase diagram of the three component, three phase systems, D_2-DT-T_2 and H_2-HT-T_2 in the region 14-21K; triple points, by calibrated temperature sensors; vapor pressure, by baratrons; gas phase equilibrium constants and kinetics by Uthe Quadrupole Mass spectrometer; liquid/solid equilibrium constants and kinetics by the nine-line fundamental infrared vibration rotation spectrum at 3-4.5μm.

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M. G. Bowman - Phone: (FTS) 843-6014 or 505 667-6014

145. HIGH TEMPERATURE MATERIALS FOR ENERGY APPLICATIONS — $250,000 — 01-02
S. S. Hecker, E. K. Storms, B. A. Mueller

Knudsen and Langmuir vaporization of various compositions near LaB_6; boron and lanthanum 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. Multiaxial mechanical testing of aluminum, copper and stainless steel properties related to microstructure by transmission and scanning electron microscopy, optical metallography and X-ray diffraction.

146. HIGH TEMPERATURE IRRADIATION DAMAGE STUDIES — $240,000 — 01-04
W. V. Green, D. M. Parkin, R. D. Brown, W. F. Sommer, J. Goldstone, M. L. Simmons, L. S. Levinson

The LAMPF accelerator, its proton beam as a radiation damage source; completion of the proton-irradiation port (PIP); uniform heavy spallation ion production; concurrent gas production; Al and Cu irradiations; voids; gas bubbles on grain boundaries; grain boundary failure at 30 dpa; damage rates of 25 dpa per day in Mo by protons; damage cross sections as function of neutron energy using internal friction; neutron irradiation effects cavity with few liters volume, flux 2.3 x 10^{13} n/cm^2s now.

LOS ALAMOS SCIENTIFIC LABORATORY (Continued)
Theoretical Division

147. LOS ALAMOS EQUATION OF STATE LIBRARY — $180,000 — 02-03
G. I. Kerley, B. I. Bennett

To set up a national library of equations of state and related material properties; will send data to interested workers and assist them to incorporate the tabular EOS methods in their hydrodynamics codes; will serve as a repository for EOS data generated by other laboratories; study EOS theories and develop better models for use in calculations; studies of melting, chemical equilibrium and electronic excitation.

Energy/Q Division

148. ULTRAHIGH PRESSURE STUDIES OF HYDROGEN — $ 80,000 — 02-02
W. Kirk, R. L. Mills

Measuring the equation of state of hydrogen and deuterium up to 40 kbar using a piston-cylinder apparatus with multistage press; effects of high pressure hydrogen impregnation on the superconductivity of palladium alloys; diamond anvil cell for studies at pressures up to 1 Mbar; optical measurements at pressure.

149. CTR RELATED CHEMICAL RESEARCH TRITIUM CHEMISTRY ASSOCIATED WITH THE LITHIUM BLANKET AND CONTAINER MATERIALS — $150,000 — 03-02
D. H. W. Carstens, W. A. Stark, J. L. Anderson - (CMB Division)

Simultaneous measurement of diffusion coefficient and solubility of T_2 in liquid Li and container materials Nb, Nb-1%Zr; development and modeling of experimental infusion technique which accounts for Sieverts' law behavior of hydrogen isotopes in metals; preliminary studies to cover the temperature range 1000 - 1400 K and a pressure range 10^{-1} - 10^4 Pa; pressure-composition-temperature diagrams of metal-hydrogen systems including alloys of Ce ($Ce_{4.5}Ni$, Ce_3Co, and $Ce_{8.5}Fe$) and of La ($La_{5.3}Ni$, La_3Ni, LaNi, and $LaNi_2$); measurements of phase diagrams of appropriate metal-tritium and alloy-tritium systems; removal of tritium from helium streams using liquid eutectic alloys.

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

150. LIQUID METALS AND SALTS FOR ENERGY SYSTEMS — $190,000 — 01-03
L. J. Wittenberg

Characterization of the liquid state of high temperature, non-aqueous inorganic materials; electrotransport phenomena in liquid lithium to obtain information for possible use in the extraction of tritium; optical properties, absorption coefficient in the visible range and emissivity in the infrared range of low melting metals, alloys and fused salts for solar photothermal applications.

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

151. CERAMICS RESEARCH $414,000 01-01
C. S. Yust, L. A. Harris,
S. L. Bennett, R. L. Beatty

Boron carbides, uranium carbides and europium compounds; structure and composition of grain boundaries in ceramics, wear, and erosion of ceramics; mechanical properties of oxide-metal composites; electron and optical studies of microstructure of coal.

152. THEORY OF THE SOLID STATE $345,000 01-01
J. S. Faulkner, G. S. Painter,
W. H. Butler, M. H. Yoo,
G. M. Stocks, B. Gyorffy,
R. O. Jones

Time and spatial distribution of radiation-producted defects; effect of elastic self-fields on equilibrium shapes of prismatic dislocations; drift flow paths, kinetics, and capture radii for point defects in such fields; KKR band theory for calculating electronic states in periodic crystals having more than one atom per unit cell; superconducting transition temperatures calculations; multiple-scattering cluster program for electronic states of clusters of Cu, Ni, Fe atoms and effects of surfaces; DVM applied to covalent compounds of interest for potential solar energy applications; CPA treatment of nonstoichiometric compounds; decohesion theory for hydrogen embrittlement; thermal and electrical transport in transition metals.

153. PREPARATION AND SYNTHESIS OF HIGH TEMPERATURE AND SPECIAL SERVICE MATERIALS $276,000 01-01
G. W. Clark, J. D. Holder,
C. F. Yen, C. B. Finch,
O. C. Kopp

Directional solidification of metal-metal oxide binary and ternary systems; development of models for heat and mass transfer during coupled solidifications; evaluation of oxide-matrix composites for high temperature applications in gas turbines, MHD devices, tool and drill components, hydrothermally grown quartz; single crystals doped with lanthanides and actinides; study of edge-defined film-fed growth process.

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

154. STABILITIES OF MICROPHASES IN HIGH TEMPERATURE STRUCTURAL MATERIALS — $ 69,000 — 01-01
J. M. Leitnaker, D. N. Braski

Composition, structure, and stability of second phases formed under nonequilibrium conditions in iron- and nickel-base alloys; metal carbides; sigma-phase; thermodynamics of multiphase systems.

155. X-RAY DIFFRACTION RESEARCH — $276,000 — 01-01
H. L. Yakel, Jr., B. S. Borie, C. J. Sparks, Jr., R. W. Hendricks, J. Lin, R. D. Carlson, E. Ricci

Structures of Eu_2O_3; diffuse x-ray and neutron scattering measurements; study of forbidden Bragg reflections in hard superconductors; small angle scattering studies of voids in irradiated materials; precipitates, porosit in coals and catalysts; inelastic resonance scattering; application of synchrotron x-radiation to study of diffraction, fluorescence, and scattering by solids.

156. DEFORMATION AND MECHANICAL PROPERTIES — $400,000 — 01-02
R. A. Vandermeer, J. C. Ogle, R. W. Carpenter, C. L. White

Relationships between structure and deformation and mechanical properties; "shape memory" effect in U-Nb-Zr alloys; stress effects on transformations from γ-stabilized uranium alloys; fracture in body-centered cubic alloys; role of grain boundaries on deformation processes; hydrogen embrittlement; embrittlement due to segregation of elements to grain boundaries.

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

157. KINETICS AND MECHANISMS OF SURFACE AND SOLID STATE REACTIONS — $507,000 — 01-03
J. V. Cathcart, R. E. Pawel, G. F. Petersen, R. A. McKee, T. S. Lundy, P. T. Carlson, R. A. Perkins

Mechanisms of alloy reaction in Fe-base alloys with mixed gases; oxidation generated stresses; structure of reaction films and mobility of elements in them; reaction of composite materials with oxygen, CO-CO_2 mixtures, methane, H_2S, and effects of other gases; Hall effect determination of carriers; theoretical and experimental studies of atomic migration in solids; interdiffusion and intrinsic diffusion in V-Ti solid solutions; chemical and tracer diffusion in Fe-Cr-Ni; hydrogen isotopes in Cr_2O_3, TiO_2, CoO, interstitial solute atom-defect interactions in Nb and TiO_2; "fast" diffusion mechanisms.

158. ENERGY TRANSPORT IN SOLIDS — $290,000 — 01-03
D. L. McElroy, R. K. Williams, J. P. Moore, T. G. Godfrey

Development and application of measurement methods for obtaining accurate physical properties data (thermal conductivity, electrical resistivity, thermopower, specific heat capacity, and coefficient of thermal expansion) from 1.2 to 2600 K; analysis of data for information on energy transport mechanisms and evaluation of theories; refractory metals; nuclear ceramics; effects of stoichiometry, cation-anion mass ratio, and (T/θ_D), on transport properties in ceramics; irradiation effects; determination of factors influencing absorptivity and emissivity in thin films; electron-phonon interactions in transition metals.

159. METALLURGY OF SUPERCONDUCTING MATERIALS — $363,000 — 01-03
C. C. Koch, D. M. Kroeger, D. S. Easton, A. DasGupta, H. C. Freyhardt

Effect of metallurgical variables on superconducting properties in Nb- and Tc-base alloys; ac loss mechanisms in Nb and A-15 compounds; fluxoid pinning in Nb-Gd, Nb-Y, Nb-Ti-Y alloys; properties of sputter deposited $Nb_{12}Al_3Ge$; development of techniques for measuring J; structures in A-15 compounds; low temperature specific heat measurements; effect of strain on superconducting properties; ternary molybdenum sulphides ($PbMo_6S_8$); $LiTi_2O_4$; methods of preparing metastable phases and measurements of their properties.

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

160. RADIATION EFFECTS $1,330,000 01-04
J. O. Stiegler, K. Farrell,
D. S. Billington, W. A. Coghlan,
N. H. Packan, L. K. Mansur,
R. W. Carpenter, E. A. Kenik,
M. B. Lewis, T. C. Reiley,
P. Jung, J. Bentley

Void and interstitial loop formation as functions of neutron fluence, spectra, and irradiation temperature; development of quantitative relationship between neutron and heavy ion bombardment; irradiation of Al, Ni, V with self ions and α-particles in Van de Graaff and ORIC; effect of composition on swelling and loss of ductility in Al and Fe-Cr-Ni systems; in situ studies by HVEM; theoretical treatment of nucleation and growth of defect clusters, kinetic effects of accelerated irradiation and stress effects of swelling; simulation of radiation creep; effects of high gas contents on structure and properties; solute segregation during irradiation; effects on phase stability; development of analytical electron microscopy; in situ HVEM studies using environmental cell with straining stage.

161. FUNDAMENTAL STUDIES IN WELDING 01-05
G. M. Goodwin

Control of weld microstructure; effect of process parameters and residual elements; phase and composition inhomogeneity; modeling of heat and mass transfer in the welding process (to start in FY 1978).

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

162. ELEMENTARY EXCITATIONS IN CONDENSED MATTER — $610,000 — 02-01
R. L. Cappelletti, W. P. Crummett, W. C. Koehler, N. Kunitomi, H. Miwa, H. A. Mook, R. M. Nicklow, H. G. Smith, Y. Tsunoda, N. Wakabayashi

Inelastic neutron scattering studies of phonons, magnons, excitons, and single particle excitations in solids and liquids; lattice dynamics and magnetic excitations in NdSb; phonon spectra of $NaClO_3$; phonons and magnetic excitations in EuO; lattice dynamics and magnetic excitations in the mixed valence systems SmS and $Sm_xY_{1-x}S$; phonons and magnons in the system Ni-Pt; inelastic scattering from noble gases; exchange interactions and anisotropy energies in rare earth-iron Laves phase compounds; spin waves in amorphous Fe and Co.

163. MAGNETIC PROPERTIES OF SOLIDS — $580,000 — 02-01
J. W. Cable, H. R. Child, L. David, W. C. Koehler, H. A. Mook, R. M. Moon, R. M. Nicklow, R. Parra

Elastic and inelastic scattering of polarized and unpolarized neutrons by magnetic systems; magnetic moment distributions in dilute and concentrated alloy systems Pd-Mn, Ni-Rh, Ni-Cu, Cr-Si, Cr-Ni; form factors and moment densities in the paramagnetic metals Sc, Ti, Y, and Nb, in EuO, in cubic Laves phase compounds and in SmS and $Sm_xY_{1-x}S$; magnetic critical scattering from Gd, Er, and EuO; magnetic form factors of Gd, Ni, and Fe from magnetovibrational scattering.

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

164. PROPERTIES OF DEFECTS, SUPERCONDUCTORS, AND HYDRIDES — $380,000 — 02-01
H. R. Child, D. K. Christen, W. C. Koehler, H. A. Mook, R. M. Nicklow, H. G. Smith, S. Spooner, P. Thorel, N. Wakabayashi

Elastic, inelastic, and small angle scattering of neutrons by superconductors, superionic conductors, metal hydrides, and metals and compounds containing interstitial defects; high resolution neutron inelastic scattering studies of perturbations of phonon spectra in Cu and Al by radiation-induced interstitials; phonon spectra of high T_c superconductors; phonon anomalies in the Mo-Re and Cr-Re systems; phonon spectra of α-U; dynamical properties of tritium in metal hydrides; energy levels of H in Zr hydrides; temperature dependence of phonons in $KCl(CN^-)$ and in the silver halides; small angle neutron scattering by voids induced in stainless steel and niobium and by fluxoid lattices in Nb and Nb-Ti alloys.

165. PHYSICAL PROPERTIES OF CERAMICS — $535,000 — 02-02
E. Sonder, J. B. Bates, Y. Chen, M. M. Abraham, J. C. Pigg, F. A. Modine, R. A. Weeks, C. Wood, H. J. Stapleton, H. T. Tohver, T. Kaneda, J. C. Wang, H. L. Engstrom

Effects of high temperature, particle and ionizing radiation on defect structures of crystalline and non-crystalline refractory materials such as MgO, Al_2O_3, $MgAl_2O_4$, and SiO_2; optical and electrical properties of refractories and solid state electrolytes; determinations of ground and excited state configurations of impurities and defects; effects of impurities and defects on radiation damage rates and electrical properties; techniques include electrical and diffusion measurements, Raman scattering, polarization modulation and Fourier transform infrared spectroscopy, optical absorption and emission, electron paramagnetic resonance, and electron-nuclear double resonance.

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

166. PHYSICAL PROPERTIES OF SUPERCONDUCTORS — $390,000 — 02-02
S. T. Sekula, B. R. Appleton, D. K. Christen, R. D. Feldman, H. R. Kerchner, R. H. Kernohan, P. Thorel, H. G. Smith

Studies of superconducting fluxoid arrays, fluxoid dynamics, and fluxoid-defect interactions in Nb-, V-, and Mo-base type II superconducting alloys and A15 compounds; dc magnetization, ac magnetic permeability, and flux-creep investigations; small angle neutron scattering by fluxoid arrays in alloys and compounds; low temperature ion damage, ion implantation, and ion backscattering in superconductors; neutron inelastic scattering investigations of high-transition-temperature superconductors.

167. RESEARCH AND DEVELOPMENT ON PURE MATERIALS — $585,000 — 02-02
J. W. Cleland, M. M. Abraham, G. C. Battle, W. E. Brundage, Y. Chen, Y. K. Chang, T. F. Connolly, C. C. Robinson, R. D. Westbrook

Initial purification, crystal growth, and characterization of research quality materials; availability and physical properties of research quality materials via the Research Materials Information Center; arc-fusion growth of pure MgO, CaO, and SrO; electron-beam float-zone growth of refractory metals Ti, V, Zr, Nb, Ta, W, Ir, and Re and their alloys; preparation of refractory metals and their alloys in rod or thin foil forms; purification and growth of single crystal Ni, Nb-1 at .% V, N-doped Nb, Fe-Cr-Ni alloys, Ni-base alloys and Mo-base alloys; float zone growth, Czochralski growth and characterization of single crystal Si; grain growth of Fe-3 at.% Si buttons; single crystal growth of Ti_3Au; preparation and synthesis of spinel ferrites.

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

168. SURFACE STUDIES AND CATALYSIS — $475,000 — 02-02
L. H. Jenkins, J. R. Noonan, J. F. Wendelken, D. M. Zehner, K. Sickafus, T. S. Noggle

Studies of clean metal surfaces which either reorder or have intraplanar spacings different from those of the bulk, using combined techniques of low energy electron diffraction (LEED) and positive ion channeling spectroscopy (PICS); LEED and Auger electron spectroscopy (AES) from "d" and "f" electron band solids; quasi-atomic structure, angular emission dependence and line shape analysis of Auger spectra; true secondary electron emission and electron energy loss (ELS) spectra variation with crystallographic effects; x-ray photoelectron spectroscopy (XPS), AES, LEED and high resolution ELS studies of chemisorbed overlayers on metal substrates; analysis of vibronic structure of adsorbate covered surfaces; examination of effects of surface electronic properties with respect to solid state aspects of heterogeneous catalysis.

169. PHOTOPHYSICAL PROCESSES OF SOLAR ENERGY CONVERSION — $425,000 — 02-02
R. F. Wood, M. M. Abraham, B. R. Appleton, J. B. Bates, J. W. Cleland, B. F. Early, B. C. Larson, T. L. Polgreen, R. D. Westbrook, R. T. Young

Characterization to determine the effects of point defects, defect clusters, dislocations, twin boundaries, stacking faults, grain boundaries, and chemical impurities in Si on electrical and optical properties; thermal neutron transmutation, diffusion, and ion implantation experiments to introduce desired carrier concentration in Si without degrading carrier mobility and lifetime; annealing of lattice damage in reactor irradiated and ion implanted Si; electrical, optical (including laser-based infrared and Raman spectroscopy), x-ray diffuse scattering, and electron paramagnetic resonance property measurements on bulk single crystal and polycrystalline Si, grain boundary compensation in polycrystalline Si by neutron transmutation doping and diffusion; fabrication of p-n junction diodes by evaporation, diffusion and ion implantation; study of factors known to degrade solar cell conversion efficiency, such as voltage factor, charge loss due to surface recombination, and deviations from ideal diode curve.

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

170. FUNDAMENTAL ASPECTS OF METAL FRACTURE — $160,000 — 02-02
S. J. Chang, J. Narayan, T. S. Noggle, S. M. Ohr

Theoretical and experimental investigations to relate phenomena of continuum fracture mechanics to microscopic physical phenomena occurring at a crack tip; in situ transmission electron microscopy.

171. ION IMPLANTATION — $ 80,000 — 02-02
B. R. Appleton, C. W. White, G. J. Clark

Ion implantation of boron into single crystal and polycrystalline NTD Si for solar cells; lattice location of implanted O in Nb; radiation damage effects associated with ion implantation; effects of ion implantation on superconducting properties of Nb.

172. THEORY OF CONDENSED MATTER — $690,000 — 02-03
R. F. Wood, M. T. Robinson, H. L. Davis, J. H. Barrett, J. F. Cooke, D. K. Holmes, T. Kaplan, M. E. Mostoller, O. S. Oen, M. Ulehla

Band structure calculations in metals and insulators; electronic properties of rare-earth and actinide compounds; 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 self-interstitials in fcc metals; 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.

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

173. LOW TEMPERATURE RADIATION EFFECTS — $475,000 — 02-04
R. R. Coltman, Jr., C. E. Klabunde, J. K. Redman, J. M. Williams

Interlaboratory program on $4^{o}K$ damage rates in V, Nb, and Mo alloys; fission-neutron damage rates at $4^{o}K$ in Cu, Ni and stainless steel; irradiation methods for neutron scattering study of $4.9^{o}K$ irradiated Cu; low-temperature recovery studies of thermal-neutron-irradiated high purity V, Mo and stainless steel; resistance and magnetoresistance measurements of fast-neutron-irradiated pure and commercial Cu; correlation of ion damage with fission-neutron damage in Al at $4^{o}K$; resistivity studies of production and recovery of damage in Cu, Nb and Pt irradiated at $4.2^{o}K$ by high energy d-Be neutrons.

174. X-RAY DIFFRACTION AND ELECTRON MICROSCOPY — $315,000 — 02-04
T. S. Noggle, S. M. Ohr, B. C. Larson, J. B. Roberto, J. Narayan, F. A. Sherrill

Radiation damage due to 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; anisotropic elasticity theory of dislocation loops; computer simulation of electron microscopy images; theory of interactions of electrons and x-rays with defects in solids.

175. ION BOMBARDMENT — $255,000 — 02-04
B. R. Appleton, O. E. Schow III, C. W. White, G. J. Clark, Q. C. Murphree, D. D. Allred

Positive ion channeling characterization of reordered surface structures of Au single crystals; characterization of stoichiometry and thickness of oxide layers on Nb single crystals by ion channeling techniques; radiative electron capture measurements as a function of path length for fully stripped oxygen ions channeled in Ag single crystals; measurements of concentration and depth distribution for hydrogen in hard Au films and in various minerals by resonant nuclear reaction techniques; characterization of hydrogen concentration and depth distributions in amorphous silicon films by resonant nuclear reaction techniques and comparison with SIMS measurements; detailed analysis of hard He ions hyperchanneled in Ag and Au thin single crystals.

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

176. NORMALIZATION OF ION AND NEUTRON DAMAGE — $135,000 — 02-04
T. S. Noggle, J. Narayan, J. M. Williams, B. R. Appleton, O. S. Oen, T. Iwata, G. Vogel

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; depth distribution of Cu and Ni ion damage in Cu and Ni; damage theory computations.

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

177. CHEMICAL STRUCTURE OF ENERGY RELATED MATERIALS — $670,000 — 03-01
W. R. Busing, G. M. Brown, C. K. Johnson, H. A. Levy, A. H. Narten, W. E. Thiessen, L. Blum

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 structures 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, macromolecular catalysts for hydrogen production, sterically hindered hydrocarbons, and compounds derived from the coal research or tertiary oil recovery programs.

178. MATERIALS CHEMISTRY RELATED TO FUSION REACTOR SYSTEMS — $430,000 — 03-02
J. T. Bell, F. J. Smith, J. D. Redman, G. M. Begun

Acquisition and interpretation of thermodynamic and kinetic data that is needed for effective tritium management in Fusion Reactor Systems is the project goal. Tritium permeabilities of metal and alloys proposed for construction of Fusion Reactor Systems are measured; permeation rates through unoxidized metals and alloys and through metals and alloys while being oxidized with steam are determined; the effects of oxide films formed by steam oxidation to impede permeation, the chemical composition and physical integrity of these oxides are of primary importance. Basic chemical information is being obtained on the behavior of tritium in materials proposed for CTR breeding blankets (e.g., molten lithium, Li_2BeF_4, and Li-Al alloy), and in materials proposed for processing tritium in the fusion fuel cycle. An example of the latter is the study of the yttrium-hydrogen isotope systems since yttrium is proposed as a tritium getter.

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

179.	PHYSICAL CHEMISTRY OF MOLTEN SALTS IN ENERGY UTILIZATION J. Braunstein, M. Furrier, C. E. Vallet, C. A. Girard	$180,000	03-03

Electrochemical techniques, thermodynamics of irreversible processes, nuclear magnetic resonance, applied to diffusion, migration, electrical conductance, relaxation mechanisms in ionic systems such as molten salts, hydrous melts, vitreous and solid electrolytes; concentration polarization in high temperature battery and fuel cell electrolytes.

180.	MOLTEN SALT FUEL CELL AND BATTERY RESEARCH J. Braunstein, C. E. Vallet, C. A. Girard	$ 50,000	03-03

Electrochemical mass transport theory, computer simulation and experimental verification of predicted composition changes in analogs of molten salt batteries and molten carbonate fuel cells.

181.	LOCALIZED CORROSION AND STRESS CORROSION CRACKING PHENOMENA RELATED TO ENERGY TECHNOLOGIES F. A. Posey, A. L. Bacarella, E. J. Kelly, A. A. Palko	$250,000	03-03

Basic electrochemical 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 (such as pitting, crevice corrosion, and stress corrosion cracking); kinetics of coupled active-passive electrode systems; kinetics of initiation of crevice corrosion, especially of titanium; effects of temperature and solution and alloy composition on pitting potentials and pit growth kinetics of metals.

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

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

182. CERAMICS FOR ENERGY APPLICATIONS — $140,000 — 01-01
R. P. Turcotte, L. C. Olsen, T. D. Chikalla

Radiation damage in fluorite crystal ceramics and glass; alpha implantation, study of structural changes and helium trapping/diffusion. Metal-insulator-semiconductor photovoltaics; Al/SiO_2/p-Si and Au/SiO_2/n-Si systems, current voltage and spectral response characteristics, surface and interface characterization by ellipsometry and Auger analysis.

183. SPUTTER-DEPOSITED SOLAR MATERIALS — $ 80,000 — 01-01
S. D. Dahlgren, R. Wang, W. T. Pawlewicz, C. H. Henager, Jr.

Effect of grain structure on the electrical transport properties of silicon; cathodic sputtering; relationships of measured carried mobility to grain structure; amorphous silicon photovoltaic properties; cathodic sputtering of photothermal absorber materials; influence of preparation technique on surface topography and solar radiation reflectance, absorption and emission; photoelectrolysis electrodes; effect of stoichiometry and microstructure on the transport properties and electrochemistry of polycrystalline ceramic photoelectrodes; influence of metallurgical variables on the transfer mechanism and on the energy barrier between the ceramic electrode and the electrolyte; fine-grained and amorphous $SrTiO_3$.

184. FUNDAMENTAL STUDIES OF STRESS CORROSION AND CORROSION FATIGUE MECHANISMS — $120,000 — 01-02
R. H. Jones, M. T. Thomas, R. E. Westerman

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 will be conducted using the Auger Electron Spectrometer for in-situ measurements of surface phenomena in gaseous environments and to relate grain boundary chemistry to intergranular fracture in aqueous environments.

PACIFIC NORTHWEST LABORATORY (Continued)

185. SPUTTER-DEPOSITED SUPERCONDUCTORS — $120,000 — 01-03
S. D. Dahlgren, R. Wang, C. H. Henager, Jr.

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, $Nb_3(Al-Ge)$, Nb_3Ge, Nb_3Sn, Nb_3Si; effect of substrate on sputter-deposited superconductor properties.

186. TRANSURANIUM PHYSICAL METALLURGY RESEARCH — $ 10,000 — 01-03
M. D. Merz, R. D. Nelson

Mechanical and physical properties of neptunium, elastic moduli, yield strnegth, work hardening; deformation mechanisms (program completed in FY 1977).

187. OXIDATION, CORROSION AND WEAR RESISTANT FINE-GRAINED MATERIALS — $120,000 — 01-03
M. D. Merz

Study of fine-grained, sputter-deposited materials; structure property relationships; ultrafine-grained and amorphous materials; basic oxidation mechanisms and kinetics in pure metals and alloys; Cu, Fe, Ni, Fe-Cr-Ni and Ni-Cr with and without oxide dispersants; diffusion of protective oxide forming elements; activation energies and rate controlling steps for oxide formation; mechanisms for formation of adherent or spalling oxides; aqueous corrosion of amorphous materials; pitting and stress corrosion mechanisms; extremely hard alloys and intermetallic components; WC, HfC and Si-B; diskrider method of wear evaluation in vacuum or controlled atmosphere; coefficient of friction; optical, SEM and TEM microscopy.

PACIFIC NORTHWEST LABORATORY (Continued)

188. RADIATION EFFECTS ON METALS — $380,000 — 01-04
J. L. Brimhall, E. P. Simonen, H. E. Kissinger, P. L. Hendrick, L. A. Charlot

Production migration and interaction of irradiation produced defects; effect of helium on void nucleation in refractory metals and high purity nickel alloys; theoretical analysis of void nucleation and growth behavior; analysis of annealing behavior in irradiated molybdenum; simulation of neutron radiation enhanced creep by light ions.

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

Examine validity of theory describing scattering of light from rough surfaces by using visible wavelengths and controllably roughened single crystal surfaces; optical scattering; controllably roughened surfaces; sample topography evaluation using modified Nomarski microscopy, examine effects of radiation damage on the optical properties of reflectors appropriate for laser fusion applications; laser fusion reflectors; radiation damage to reflectors; copper reflectors; in-situ measurements of mirror optical properties during irradiation.

190. SPUTTER-DEPOSITED COATINGS FOR OPTICAL APPLICATIONS — $ 80,000 — 02-02
N. Laegreid, W. T. Pawlewicz, D. D. Hays, R. Busch

Development of sputter-deposited materials for optical applications, TiO_2, SiO_2, ZrO_2, HfO_2, Ta_2O_5 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 bond edge by normal incidence transmission and reflection, x-ray energy spectrometry, x-ray diffraction, scanning electron microscopy and transmission electron microscopy.

SANDIA LABORATORIES (ALBUQUERQUE)
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Albuquerque, New Mexico 87115

A. Narath - Phone: (FTS) 475-4673 or 505 264-4673
J. Galt - Phone: (FTS) 473-4669 or 505 264-4669

191. Stress Corrosion Cracking — $ 70,000 — 01-02
W. H. Smyrl, M. Davis

Crack propagation behavior of austenitic and ferritic stainless steels in molten salt environments; low melting mixtures of $AlCl_3$-NaCl-KCl-LiCl; molten salt has been chosen to provide data at the same temperature and pressure as have been used in boiling aqueous $MgCl_2$ solutions; electrochemical investigations to be conducted in parallel with the stress corrosion tests; reactions will be studied with pulse and alternating current impedance techniques.

192. ION IMPLANTATION AND DEFECTS IN MATERIALS — $150,000 — 01-03
K. L. Brower, D. M. Follstaedt, G. B. Krefft, S. M. Myers, C. B. Norris, F. L. Vook, P. S. Peercy, S. T. Picraux

The application of ion-beam techniques to studies of surface phenomena insulators, semiconductors, and metals; ion implantation investigations in MgO; cathodoluminescence measurements in GaAs, CdTe; optical absorption, Rutherford backscattering channeling, and channeled proton induced x-ray measurements in ion damaged Al_2O_3; ion implantation modification of near surface region in lithia-alumina-silica glasses; ion implantation and ion backscattering analysis to determine phase boundaries and diffusion rates in Be and Fe systems.

193. SURFACE PHYSICS RESEARCH — $190,000 — 02-02
J. E. Houston, J. A. Panitz, R. R. Rye, P. J. Feibelman, F. L. Vook

Applications of field desorption mass spectrometric techniques to the problem of imaging molecules during their interaction with solid surfaces; desorption studies of benzene adsorbed on tungsten surfaces; construction of a low temperature field desorption spectrometer; electron spectroscopic lineshape analyses of adsorption and gas-phase systems.

SANDIA LABORATORIES (ALBUQUERQUE) (Continued)

194. HYDROGEN PRODUCTION BY SOLAR-PHOTOASSISTED ELECTROLYTIC DECOMPOSITION OF WATER — $100,000 — 02-02

M. A. Butler, D. S. Ginley, M. L. Knotek, B. Morosin, J. E. Schirber

To investigate the economic feasibility of H production by photo-assisted electrolysis of H_2O at chemically inert semiconductor electrodes; electrochemical studies; variation of semiconductor electrode material properties; surface studies; theoretical studies to model the behavior devices; WO_3 and TiO_2.

SANDIA LABORATORIES (LIVERMORE)
Livermore, California 94550
A. Narath - Phone: (FTS): 475-4673 or 505 264-4673
B. Murphey - Phone: (FTS): 469-2884 or 415 455-7011

195. GASES IN METALS $140,000 01-02
G. J. Thomas, W. D. Wilson,
W. A. Swansiger, C. F. Melius,
W. R. Hoover

Experimental and theoretical studies of H and He in solids; diffusion, trapping and clustering of He introduced by T decay; theoretical calculations of the activation energy for He migration and energies of He binding to simple defects; uniaxial tensile testing to study He embrittlement, transmission electron microscopy; nickel, refractory metals, stainless steel.

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.

UNIVERSITY OF ARIZONA

201. STUDY OF GAS EVOLUTION THRESHOLDS AT SEMICONDUCTOR-ELECTROLYTE INTERFACES USING DIFFERENTIAL REFLECTANCE SPECTROSCOPY — $67,110 — 02-02
S. Sari - Optical Sciences Center

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 will be studied.

ARIZONA STATE UNIVERSITY

202. IMAGING SURFACES AND DEFECTS IN CRYSTALS — $77,909 — 02-02
J. M. Cowley - Dept. of Physics

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.

BROWN UNIVERSITY

203. A COMBINED MACROSCOPIC AND MICROSCOPIC APPROACH TO THE FRACTURE OF METALS — $110,000 — 01-02
J. Gurland and J. R. Rice - Division of Engineering

Analysis of ductile fracture of metal, crack initiation and growth and shear localization; experimental studies of these phenomena in steels; effects of second phase distribution, dislocation arrays, and grain and subboundaries; hydrogen and impurity (temper) embrittlement; techniques used-mechanical testing, quantitative metallography, finite element and crystal plasticity modeling.

UNIVERSITY OF CALIFORNIA/LOS ANGELES

204. HIGH TEMPERATURE IRRADIATION DAMAGE OF Ni-BASE ALLOYS — 70,002 — 01-04
A. J. Ardell - Dept. of Materials

Effects of solute additions on irradiation induced defect formation in Ni-base alloys at elevated temperatures; void formation in Ni-base alloys containing up to 8 at. % Al and Ti, and up to 16 at. % Cr, using 4 MeV N^+ and Ni^+ ions to 20 dpa in the temperature range 400 to 650°C; irradiation induced gamma-prime precipitation in Ni-Si alloys with up to 8 at. % Si.

UNIVERSITY OF CALIFORNIA/LOS ANGELES (Continued)

205. SEMICONDUCTOR EUTECTICS FOR ENERGY CONVERSION — $48,401 — 02-02
A. S. Yue - Materials Department

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.

UNIVERSITY OF CALIFORNIA/RIVERSIDE

206. THEORETICAL ASPECTS OF SUPER-CONDUCTOR BEHAVIOR — $47,000 — 02-03
E. Simanek - Physics Department

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

207. THE RESPONSE OF SUPERCONDUCTORS TO VARIATIONS IN IMPURITY CONTENT AND APPLIED PRESSURE — $186,436 — 02-02
M. B. Maple - Dept. of Physics

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 Tc superconductors.

208. RESEARCH ON THE PROPERTIES OF MATERIALS AT VERY LOW TEMPERATURES — $221,668 — 02-02
J. C. Wheatley - Dept. of Physics

The orbital properties of superfluid ^{3}He-A are some of the most novel properties of this new superfluid. In our new work we will study both the cause and nature of the persistent orbital motions discovered last year and the orbital response following sudden changes in a magnetic field. We are also studying the anomalous static magnetism in ^{3}He-B and the nature of spin relaxation in both the A and B phases.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA

209. RESONANCE STUDIES OF SUPERIONIC CONDUCTORS — $64,061 — 02-02
V. Jaccarino - Physics Department

NMR and EPR study of superionic and related compounds; use of magnetic ions as a probe of activated motion; use of fast decay of the electronic spin correlation functions in magnetically dense compounds to probe activated hopping in the 10^{-11} to 10^{-12} sec. time domain; 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.

CALIFORNIA INSTITUTE OF TECHNOLOGY

210. STUDIES OF ALLOY STRUCTURES AND PROPERTIES — $145,000 — 01-01
P. Duwez - Division of Engineering

Structure and properties of new metastable amorphous alloys obtained by rapid cooling from the liquid state; magnetic and superconducting properties of amorphous alloys; one class of alloys being studied for their magnetic properties contain 75% of transition metals (Ni, Co, Fe, Mn) and 25% of metalloids (B, C, Si or P); another class of alloys being studied for their superconducting properties contain two metals such as La-Au or Gd-Au; methods for introducing fine quasi-crystalline precipitates into metallic glasses.

211. THE PRESSURE DEPENDENCE OF THE MECHANICAL PROPERTIES OF POLYMERS — $39,200 — 01-02
N. W. Tschoegl - Dept. of Chemistry and Chemical Engineering

Development of pressure-time-temperature superposition principle for elastomers. Measurement of shear moduli, thermal expansivity, and compressibility under pressure up to 10 kbars; analysis of behavior near glass transition pressure.

212. A STUDY OF METAL HYDRIDES AND IONIC CONDUCTORS WITH NUCLEAR MAGNETIC RESONANCE TECHNIQUES — $75,000 — 03-01
R. W. Vaughan - Chemistry and Chemical Engineering Dept.

Multiple pulsed nuclear magnetic techniques to investigate chemical and electronic bonding in binary metal hydrides. Materials to be studied include the alkaline-earth hydrides, group IVA hydrides, particularly titanium and zirconium hydrides, and the group VIII hydride, palladium hydride.

CARNEGIE-MELLON UNIVERSITY

213. KINETICS, MORPHOLOGY AND THERMODYNAMICS OF THE SOLID-LIQUID TRANSITION OF NON-METALS — $40,000 — 01-01
R. F. Sekerka - Dept. of Metallurgy and Materials Science

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.

CASE WESTERN RESERVE UNIVERSITY

214. STUDY COUPLED DIFFUSION PHENOMENA IN MULTICOMPONENT GLASSES AND GLASS FORMING LIQUIDS — $51,500 — 01-03
A. R. Cooper - Dept. of Metallurgical and Materials Sciences

Multicomponent diffusional mass transport in both temperature and concentration gradients; theoretical and experimental; chemical potentials; intrinsic and chemical diffusion coefficients; glasses and glass forming liquids; $K_2O \cdot SrO \cdot SiO_2$ system.

215. ENVIRONMENTAL REACTIONS AND THEIR EFFECTS ON MECHANICAL BEHAVIOR OF METALLIC MATERIALS — $64,800 — 01-02
R. Gibala - Division of Metallurgy and Materials Science

Investigation of surface oxide films and interstitial clustering (H-O and D-O) on the yield and flow of refractory metals, principally Nb and Ta alloys; strengthening mechanisms; solute partitioning to defects; techniques used-mechanical testing, electrical resistivity, in-situ high voltage electron microscopy.

216. PLASTIC DEFORMATION IN OXIDE CERAMICS — $59,715 — 01-02
A. H. Heuer - Dept. of Metallurgical and Materials Sciences

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 annhilation kinetics and determine diffusion coefficients.

CASE WESTERN RESERVE UNIVERSITY (Continued)

217. EXPERIMENTS IN HIGH VOLTAGE ELECTRON MICROSCOPY — $78,115 — 01-04
T. E. Mitchell - Division of Metallurgy and Materials Science

High voltage electron microscopy of in-situ radiation damage and kinetic process enhancement; displacement energies in copper, chromium, stainless steel, and vanadium; enhanced precipitation in aluminum-copper, aluminum-silicon, and nickel-aluminum alloys; void and dislocation loop formation in copper and nickel; displacement damage in quartz, aluminum oxide, and magnesium oxide.

218. ELASTIC AND PLASTIC STRAINS AND THE STRESS CORROSION CRACKING OF AUSTENITIC STAINLESS STEELS — $39,400 — 01-02
A. R. Troiano - Division of Metallurgy and Materials Science

Study of stress corrosion cracking of transformable and non-transformable austenitic stainless steels in aqueous cloride solutions; evaluation of prior plastic strain and residual stress on electrochemical potentials for pitting, cracking and corrosion.

UNIVERSITY OF CHICAGO

219. THE STUDY OF PHONONS AND ELECTRONIC PROCESSES IN ORDERED AND DISORDERED SOLIDS — $61,000 — 02-02
S. A. Solin - Dept. of Physics

Raman, infrared and x-ray techniques used to investigate irreversible and reversible photostructural and thermostructural transformations in bulk As_2O_3 glass. The atomic configurations associated with these transitions are investigated in detail. Superhard thin films of amorphous diamonds are studied with Raman spectra to relate the microstructural film features to important physical parameters.

UNIVERSITY OF CINCINNATI

220. FLUX PINNING AND FLUX FLOW STUDIES IN SUPERCONDUCTORS USING FLUX FLOW NOISE TECHNIQUES — $49,909 — 02-02
W. C. H. Joiner - Dept. of Physics

The objective of this work is to study flux pinning and the dynamics of flux flow in type II syperconductors. 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.

UNIVERSITY OF CINCINNATI (Continued)

221. RADIATION EFFECTS TO BCC REFRACTORY METALS AND ALLOYS — $45,000 — 01-04
J. Moteff - Dept. of Materials Science and Metallurgical Engineering

Microstructure and high temperature strength of refractory metals (Mo and Nb alloys); comparison of neutron and heavy ion effects; techniques used-hot hardness, creep, electrical resistivity, transmission electron microscopy.

UNIVERSITY OF COLORADO

222. CRITICAL SCATTERING OF LASER LIGHT BY BULK FLUIDS AND THIN FLUID FILMS — $66,070 — 02-02
R. Mockler and W. O'Sullivan - Dept. of Physics and Astrophysics

The dependence upon film thickness of the critical temperature of binary fluid films will be studied using index of refraction techniques. The cross-over from three-dimensional Ising model to mean field behavior observed in critical fluid films for thicknesses $\leq$ 10μm will be studied to determine if there is an intermediate scaling region. Intensity auto correlation studies will be made of the Rayleigh line width dependence on film thickness for critical fluid films.

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

223. HYDROGEN AND METHANE SYNTHESES THROUGH RADIATION CATALYSIS — $161,990 — 02-02
J. G. Morse, Colorado School of Mines
J. DuBow, Colorado State University

Ionizing radiation has been shown to increase reaction rates by up to two orders of magnetude. 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

224. LIQUID LITHIUM CORROSION AND CORROSION-FATIGUE RESEARCH — $89,564 — 01-01
D. L. Olson and D. K. Matlock
Dept. of Metallurgical Engineering

Chemical and mechanical degradation of ferrous alloys in contact with liquid reactive metals; grain boundary penetration and weight loss kinetics of stainless steel in liquid lithium as a function of temperature and nitrogen concentration; activation energies associated with corrosion processes; effect of nitrogen getters; Mossbauer spectroscopy, scanning electron microscopy, Auger electron spectroscopy) and contact potential measurements.

COLUMBIA UNIVERSITY

225. HIGH TEMPERATURE TRANSPORT PROPERTIES AND PROCESSES OF GASES AND ALKALI METALS — $46,000 — 03-02
C. F. Bonilla - Dept. of Chemical Engineering

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

226. ELECTRODE POLARIZATION STUDIES IN HOT CORROSION SYSTEMS — $46,500 — 01-01
O. F. Devereux - Dept. of Metallurgy

Investigation of corrosion of metals (Fe, steels) in mixed gases and in molten salts (specifically Na_2CO_3) containing activities of H, S, O, and C selected to simulate coal conversion processes; high temperature polarization curves; corrosion kinetics.

227. ELECTRON-DISLOCATION INTERACTIONS AT LOW TEMPERATURES — $45,466 — 01-02
J. M. Galligan - Dept. of Metallurgy

Electron 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; Pb, Pb-Sn, Pb-Ag, Cu and Nb.

228. CLUSTER CARBURIZING — $39,800 — 01-01
J. E. Morral - Dept. of Metallurgy
and Inst. of Materials Science

Experimental study of transformation of precipitates during carburization of refractory metal (Nb and Ta) alloys; analysis of carbon partitioning and its effect on phase equilibria.

CORNELL UNIVERSITY

229. INFLUENCE OF GRAIN BOUNDARIES ON THE ELECTRICAL TRANSPORT PROPERTIES OF POLYCRYSTALLINE Si FILMS — $45,800 — 01-01
D. G. Ast - Dept. of Materials Science and Engineering

Measurements and modelling of structure of and impurity distribution and at grain boundaries in pure and doped silicon, using transmission microscopy analysis, electron beam induced current to evaluate effect to defects on electrical properties near boundaries, and Lang x-ray topography to characterize macrodistribution of defects and boundaries.

230. STRUCTURE AND PROPERTIES OF GRAIN BOUNDARIES — $92,743 — 01-01
R. W. Balluffi - Dept. of Materials Science and Engineering

Theoretical and experimental investigation of the structure and properties of grain boundaries in metals; use of thin film specimens containing boundaries of controlled geometry; x-ray diffraction studies of grain boundary structure; diffusion along grain boundaries; faceting and preferred crystal orientation of grain boundaries; Au alloys; Auger electron spectroscopy and electron microscopy.

231. REDUCTION OF MIXED SPINEL OXIDES — $58,786 — 01-01
L. C. DeJonghe - Dept. of Materials Science and Engineering

Reduction kinetics and related microstructural changes of oxide spinels by hydrogen; Fe_3O_4, $CoFe_2O_4$, and $NiFe_2O_4$; effects of MgO and Al_2O_3 substitutions; thermogravimetric analysis and transmission electron microscopy.

232. ENVIRONMENT AND FRACTURE — $67,350 — 01-02
H. H. Johnson - Dept. of Materials Sciences and Engineering

Evaluation of hydrogen permeation into metals (Nb, Fe, steels); partitioning to defects such as second phases, pores, and dislocations; effect on hydrogen embrittlement (steels) and hydride stability (Nb).

233. INELASTIC DEFORMATION IN NON-METALLIC CRYSTALLINE SOLIDS — $45,000 — 01-02
D. L. Kohlstedt - Dept. of Materials Science and Engineering

Plastic deformation of transition metal carbides; load relaxation, constant strain rate and creep experiments; transmission electron microscopy; correlation of dislocation substructures to a mechanical equation of state.

CORNELL UNIVERSITY (CONTINUED)

234. MECHANICAL BEHAVIOR OF MATERIALS AND STRUCTURAL ELEMENTS AT ELEVATED TEMPERATURES — $74,000 — 01-02
R. H. Lance and E. W. Hart - Dept. of Theoretical and Applied Mechanics

Analytical and experimental research on the mechanical behavior of structural elements at elevated temperatures; solutions of boundary value problems involving time varying loads using generalized constitutive relations; creep testing of beams, plates and shells at room and elevated temperature.

235. MECHANICAL PROPERTIES OF CRYSTALLINE SOLIDS — $81,000 — 01-02
C-Y. Li - Dept. of Materials Science and Engineering

Mechanical properties of crystalline solids investigated using a plastic equation of state approach; to generate information for mechanical testing and mechanical design at elevated temperatures; techniques used include tensile, load relaxation, anelastic deformation testing; stainless steel, nickel, zircalloy, lead.

236. PROBABILISTIC MODELS OF THE STRESS-RUPTURE OF COMPOSITE MATERIALS — $49,100 — 01-02
S. L. Phoenix - Sibley School of Mechanical and Aerospace Engineering

Modelling of time-dependent strength of fiber-reinforced polymer matrix composites; effect of fiber fracture statistics, composite size, and matrix viscoelastic behavior.

237. HIGH TEMPERATURE MECHANICAL BEHAVIOR OF SILICON NITRIDE UNDER TRANSIENT LOADING — $36,000 — 01-02
R. Raj - Dept. of Materials Science and Engineering

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

CORNELL UNIVERSITY (CONTINUED)

238. DEFECTS IN METAL CRYSTALS — $195,000 — 01-04
D. N. Seidman - Dept. of Materials Science and Engineering

Properties of self-interstitial atoms, aggregates of self-interstitial atoms, interaction with solute atoms, non-equilibrium segregation of solute atoms to voids, migration energy of interstitial helium in tungsten, range of helium in tungsten, range of focusing collision sequences in pure metals and ordered alloys; field ion microscopy, atom-probe field-ion radiation, electron microscopy; transmission sputtering of Au; depleted zones in Pt-Au; effect of N on self ion damage in Ta; void formation in stainless steel.

DREXEL UNIVERSITY

239. STRAIN HARDENING AND DUCTILITY OF IRON: AXISYMMETRIC VS. PLANE STRAIN ELONGATION — $43,400 — 01-02
G. Langford - Dept. of Materials Engineering

Characterization of dislocation configurations in and resultant strain hardening of iron during deformation processes-wire drawing, strip drawing, and a combination of these.

DARTMOUTH COLLEGE

240. THEORY OF ELECTRON-PHONON SCATTERING EFFECTS IN METALS — $35,784 — 02-03
W. E. Lawrence - Dept. of Physics and Astronomy

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

241. EXPERIMENTAL DETERMINATION OF THE TEMPERATURE DEPENDENCE OF METALLIC WORK FUNCTIONS AT LOW TEMPERATURES — $33,808 — 02-02
P. B. Pipes - Dept. of Physics and Astronomy

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.

UNIVERSITY OF FLORIDA

242. QUANTITATIVE ANALYSIS OF SOLUTE SEGREGATION IN ALLOYS BY TRANSMISSION ELECTRON MICROSCOPY — $52,000 — 01-01
J. J. Hren and C. S. Hartley - Dept. of Metallurgical and Materials Engineering

Study of transmission electron microscopy images - their simulation and experimental observation; effects of solute strain fields and anisotropic elasticity considerations on dislocation loop images.

243. DEFORMATION PROCESSES IN REFRACTORY METALS — $42,000 — 01-02
R. E. Reed-Hill - Dept. of Materials Science and Engineering

Measurement as dynamic strain aging in Nb containing O and H; assessment of dislocation-impurity interactions and kinetics thereof; analysis of alloy work-hardening behavior; techniques used-internal friction, mechanical tests, transmission electron microscopy.

GEORGIA INSTITUTE OF TECHNOLOGY

244. THE STRUCTURE AND REACTIVITY OF HETEROGENEOUS SURFACES AND STUDIES OF THE GEOMETRY OF SURFACE COMPLEXES — $83,619 — 02-03
U. Landman and E. W. Montroll - Department of Physics

This is an investigation of methods for the study of the geometry of surface atomic environments - in particular the EXAFS-Auger method. In addition a development of techniques of characterization of complex surface systems via the heterogeneous response site distribution method will be carried out.

245. INVESTIGATIONS OF RELATIONSHIPS BETWEEN MICROSTRUCTURE, MAGNETIC PROPERTIES AND THE HYDRIDING PROCESSES IN INTERMETALLIC COMPOUNDS OF RARE EARTH AND TRANSITION METALS — $78,672 — 01-01
B. R. Livesay - Applied Sciences Laboratory

Correlations between microstructure, chemical composition and physical properties of selected intermetallic compounds as a function of hydrogen sorption and desorption processes; FeTi, RT_5 (R = rare earth metal, T = transition metal); effect of ternary elements; hydride nucleation sites, growth mechanisms; hydride decomposition, hysteresis and stability; TEM, AES, SEM and magnetic property measurement.

UNIVERSITIES

UNIVERSITY OF HAWAII

246. PRESSURE DERIVATIVES OF ELASTIC MODULI IN B.C.C. TRANSITION METALS AND THEIR SOLID SOLUTIONS — $41,921 — 02-02
M. H. Manghnani - Dept. of Geology and Geophysics

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.

247. PHOTOELECTRIC EMISSION FROM THIN FILMS IN THE VACUUM ULTRAVIOLET REGION — $32,996 — 02-02
W. Pong - Dept. of Physics and Astronomy

The proposed research involves measurements of photo-emission and optical spectra of solid surfaces and thin films using dispersed ultraviolet radiation of energies 7-27 eV. The materials being looked at are alkali and alkaline-earth halides, oxides, nitrides and organic semi-conductors. The spectra provide information on density-of-states structures, band-widths, band threshholds and excitons.

UNIVERSITY OF HOUSTON

248. MICROSTRUCTURAL STUDIES OF HYDROGEN AND OTHER INTERSTITIAL DEFECTS IN BCC REFRACTORY METALS — $74,200 — 02-02
S. C. Moss - Dept. of Physics

Hydrogen (or deuterium) related phenomena (lattice strain, hydride precipitation, electronic effects-Fermi surface determination, phonon dispersion) in refractory metals (V, Nb, Ta) studied using neutron scattering, x-ray diffraction, γ-ray Compton scattering, and positron annihilation.

ILLINOIS INSTITUTE OF TECHNOLOGY

249. DIFFUSION MECHANISMS AND DEGRADATION OF ENVIRONMENTALLY SENSITIVE COMPOSITE MATERIALS — $43,400 — 01-02
L. J. Broutman - Dept. of Metallurgy and Materials Engineering

Experimental and analytical study of moisture diffusion in glass-fiber reinforced polymer composites; effect of stress on moisture permeation and primary diffusion paths; moisture effects on fatigue properties of composites.

ILLINOIS INSTITUTE OF TECHNOLOGY (CONTINUED)

250. ELECTROCHEMISTRY OF ACETYLIDES, NITRIDES AND CARBON CATHODES IN MOLTEN HALIDES — $40,000 — 03-03
J. R. Selman - Dept. of Chemical Engineering

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 subtrates and deposits.

LEHIGH UNIVERSITY

251. PRESSURE SINTERING AND CREEP DEFORMATION - A JOINT MODELLING APPROACH — $49,005 — 01-01
M. Notis - Dept. of Metallurgy and Materials Sciences

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; CaO, NiO, and $MgAl_2O_4$

UNIVERSITY OF MARYLAND

252. AN INVESTIGATION OF IRRADIATION STRENGTHENING OF BCC METALS AND SOLID SOLUTIONS — $53,000 — 01-02
R. J. Arsenault - Dept. of Chemical Engineering

Determination of irradiation-induced defects on refractory metals, specifically yield and flow behavior of vanadium containing various oxygen impurity levels and effect of helium on high temperature behavior of niobium.

253. ALLOY STRENGTHENING DUE TO ATOMIC ORDER — $43,600 — 01-02
M. J. Marcinkowski - Dept. of Mechanical Engineering

Mathematical analysis of deformation and crack formation and growth, based on continuum elasticity representation of dislocation strain fields; recent emphasis on single dislocation interactions with holes and other dislocation arrays.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

254. MICROMECHANICAL MODELLING OF MICROSTRUCTURAL DAMAGE AT ELEVATED TEMPERATURE DURING CREEP OF SUPER-ALLOYS FOR ENERGY APPLICATIONS — $136,600 — 01-02
A. S. Argon and F. A. McClintock - Dept. of Mechanical Engineering)

Experimental and analytical study of crack initiation and growth in stainless steel and fiber-reinforced nickel alloys at high temperatures, with emphasis on particle matrix decohesion effects on creep-rupture.

255. HIGH TEMPERATURE PROPERTIES AND PROCESSES IN CERAMICS — $115,000 — 01-03
H. K. Bowen and B. J. Wuensch - Dept. of Ceramics

Mass transport behavior in ceramics; thermomigration theory and experiment; oxygen tracer diffusion; kinetic and thermodynamic factors; FeO, $FeAl_2O_4$ - Fe_3O_4 solid solutions, UO_2, UO_2-CeO_2 solid solutions, ion microprobe analysis of oxygen diffusion, Al_2O_3.

256. THE LUMINESCENCE PROCESS IN CHEMICAL REACTIONS — $61,000 — 03-03
J. L. Gole - Dept. of Chemistry

Investigations of small metallic clusters produced at temperatures above 2000°C. Characterization of metal carbides MC and MC_2, and of metal sulfides MS produced in single collision oxidation. Laser induced excitation, photoluminescence spectroscopy and mass spectrometric techniques are employed.

257. PROCESSING STUDIES OF POWDER METALLURGICALLY PRODUCED HIGH TEMPERATURE ALLOYS — $40,500 — 01-02
N. J. Grant - Dept. of Materials Science and Engineering

Powder metallurgy fabrication of nickel alloys and stainless steels; evaluation of processing and microstructure, and correlation of these with dominant strengthening mechanisms; emphasis on high temperature stress-rupture behavior of alloys containing a fine oxide dispersion. Techniques used-atomization, mechanical testing, transmission and scanning electron microscopy.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (CONTINUED)

258. BASIC RESEARCH IN CRYSTALLINE AND NONCRYSTALLINE CERAMIC SYSTEMS — $430,000 — 01-01
W. D. Kingery and R. L. Coble - Dept. of Materials Science and Engineering

Electrical, optical and dielectric properties; microstructure development during processing and evolution in service; kinetic studies of ion transport; defect interactions; solute distributions; grain boundary phenomena; optical absorption in Fe doped Al_2O_3; liquid phase sintering of CaF_2-NaF; solid solubility of SiO_2 and ZrO_2 in MgO; analytical studies of final stage sintering; defects in MgO; TEM observations of the alpha-beta transition in quartz; creep at low stresses; processing of covalent bonded materials (Si).

259. LOW TEMPERATURE AND NEUTRON PHYSICS STUDIES — $109,460 — 02-01
C. G. Shull - Dept. of Physics

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

260. ELECTRONIC CONDUCTION IN SOLID OXIDE ELECTROLYTES — $55,000 — 03-03
H. L. Tuller - Dept. of Materials Science and Engineering

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 Th O_2 examined for electronic conductivity thermoelectric power, and ionic transference number. Microstructural studies of second phases, grain boundary effects and segregation.

MICHIGAN TECHNOLOGICAL UNIVERSITY

261. A STUDY OF GRAIN BOUNDARY SEGREGATION USING THE AUGER ELECTRON EMISSION TECHNIQUE — $56,617 — 01-02
D. F. Stein and L. A. Heldt - Dept. of Metallurgical Engineering

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 brasses; hydrogen embrittlement of copper alloys and pure iron.

UNIVERSITY OF MINNESOTA

262. EXPERIMENTAL INVESTIGATIONS IN SOLID STATE AND LOW TEMPERATURE PHYSICS — $186,772 — 02-02
A. M. Goldman and W. V. Weyhmann W. Zimmermann, Jr., - Dept. of Physics

The proposed research consists of a program which includes studies of superconductivity, magnetism in metals and properties of liquid helium. The research on superconductivity is aimed at understanding the dynamics of the order parameter and fluctuations associated with the superconducting to normal transition. In the magnetism research nuclear orientation and SQUID magnetometer techniques are being used to study Kondo systems at very low temperatures. The research on liquid Helium consists of studies of the lambda transition and too critical point in liquid ^{3}He/^{4}He mixtures and of the quantum properties of the flow and rotation of the superfluid component of liquid ^{4}He.

CITY UNIVERSITY OF NEW YORK

263. NONADIABATIC APPROACH TO VIBRONICALLY ASSISTED RADIATION AND RADIATIONLESS TRANSITIONS — $53,344 — 02-03
M. Lax - Dept. of Physics

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.

STATE UNIVERSITY OF NEW YORK/STONY BROOK

264. APPLICATIONS OF MICRODYNAMICS AND LATTICE MECHANICS TO PROBLEMS IN PLASTIC FLOW AND FRACTURE — $50,500 — 01-02
J. C. Bilello - Dept. of Materials Sciences

Investigation of deformation and fracture in refractory metals (W and Mo); plastic relaxation at cracks; effects of substitutional solutes (Nb) and interstitial impurities (O) in Mo; techniques used-mechanical testing, scanning electron microscopy, etch pit mapping.

265. PREPARATION, CHARACTERIZATION AND USE OF METAL HYDRIDES FOR FUEL SYSTEMS — $44,571 — 01-01
P. J. Herley - Dept. of Materials Science

Effects of solid catalysts and gaseous environments on the thermal decomposition kinetics of aluminum hydride powder; effects of gamma-ray preirradiation; photodecomposition with high intensity u-v light; activation energies and chemical order of reactions; lithium aluminum hydride, magnesium hydride also; mechanisms underlying decomposition reactions.

266. THEORETICAL STUDIES OF CHEMISORPTION ON TRANSITION METAL SURFACES: INTERACTION OF HYDROGEN WITH TITANIUM — $69,977 — 02-03
J. L. Whitten, J. D. Doll - Dept. of Chemistry

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.

NORTH CAROLINA STATE UNIVERSITY

267. SORPTION OF CESIUM BY GRAPHITES AT HIGH TEMPERATURES — $40,000 — 03-03
L. Zumwalt - Dept. of Nuclear Engineering

Quantitative thermodynamic studies of the sorption behavior of volatile fission product metals on nuclear grade graphite; cesium sorption isotherms on strontium- and barium-impregnated graphite at a series of concentrations from 0 to 1 monolayer Sr/Ba in the temperature range 750 to 1100°C and at Cs equilibrium vapor pressures ranging from 10^{-9} to 10^{-4} atmospheres.

NORTHEASTERN UNIVERSITY

268. STUDIES OF DISLOCATION MOTION AND SLIDING FRICTION — $44,839 — 02-03
J. Sokoloff - Dept. of Physics

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.

NORTHWESTERN UNIVERSITY

269. EFFECT OF POINT DEFECTS ON MECHANICAL PROPERTIES OF METALS — $56,600 — 01-04
M. Meshii - Dept. of Materials Sciences

Experimental study of yield and flow behavior of ductile materials (Fe, Nb), effects of surface films (Ni coated Fe), self interstitials (induced by electron irradiation), impurities, crystallographic orientation.

270. BASIC RESEARCH ON CERAMIC MATERIALS FOR ENERGY STORAGE AND CONVERSION SYSTEMS — $65,000 — 01-01
D. H. Whitmore - Dept. of Materials Science

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; mixed chlorides; lithium titanates, indium and thallium ternary iodides.

UNIVERSITY OF NOTRE DAME

271. PORE SHRINKAGE AND OSTWALD RIPENING IN METALLIC SYSTEMS — $50,000 — 01-01
G. C. Kuczynski, C. W. Allen - Dept. of Metallurgy Engineering and Materials Sciences

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 alloys.

OHIO STATE UNIVERSITY

272. FUNDAMENTAL STUDIES OF METAL FLUORINATION REACTIONS — $58,100 — 01-03
R. Rapp - Dept. of Metallurgical Engineering

Experimental studies of fluorine diffusion and solubility in metals (Cu and Ni) and defects structures in fluoride electrolytes (NiF_2, PbF_2, and CaF_2); construction of an electrochemical probe to measure fluorine activity in gas mixtures.

273. HYDROGEN ATTACK OF STEEL — $40,417 — 01-02
P. G. Shewmon - Dept. of Metallurgical Engineering

Experimental investigation of the microscopic processes which limit the nucleation and growth of methane bubbles during hydrogen attack of steels; effects of microstructure, inclusions, deoxidation and alloying; metallography of fracture surfaces and volume change kinetics.

274. CORROSION, STRESS CORROSION CRACKING, AND ELECTROCHEMISTRY OF THE IRON AND NICKEL BASE ALLOYS IN CAUSTIC ENVIRONMENTS — $70,000 — 01-01
R. W. Staehle and A. K. Agrawal - Dept. of Metallurgical Engineering

Experimental determination of effect of inhibitors on electrochemical polarization curves and cracking suceptibility of steels on aqueous caustic environments; corrosion and passivation kinetics of Ni and Fe.

OKLAHOMA STATE UNIVERSITY

275. ELECTRONIC STRUCTURE OF DEFECTS IN OXIDES — $25,000 — 02-02
G. P. Summers - Dept. of Physics

Optical measurements in oxides; effects of transition metal impurities on photoconductivity of Al_2O_3; neutron-irradiation induced changes in photoconductivity, fluorescence, and absorption in CaO and SiO; determination of primary current carriers; defect electronic structure.

UNIVERSITY OF PENNSYLVANIA

276. ELECTROCHEMICAL INVESTIGATION OF NOVEL ELECTRODE MATERIALS — $69,000 — 03-02
W. L. Worrell - Dept. of Metallurgy and Materials Science

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.

PENNSYLVANIA STATE UNIVERSITY

277. CERAMIC RESEARCH — $37,070 — 01-02
R. C. Bradt and J. H. Hoke
Dept. of Materials Science

Transformational and isothermal superplasticity in two phase eutectoid systems such as Bi_2O_3 - Sm_2O_3 and in single phase Bi_2WO_6-type compounds; effects of stoichiometry on fracture and elastic properties of TiO_{2-x}, FeO_{1+x} and $MgAl_2O_4$ spinel.

278. STUDIES OF MECHANICAL PROPERTIES AND IRRADIATION DAMAGE NUCLEATION OF HTGR GRAPHITES — $31,900 — 01-04
P. A. Thrower - Dept. of Materials Science

Oxidation of graphite with various filler: binder ratios and in impure He containing CO_2, CO, and H_2 levels and at various gas flow rates; determination of microstructural degradation during oxidation and residual strength; irradiation-induced defects in boron-doped graphite.

279. STRUCTURE OF GLASSES CONTAINING TRANSITION METAL IONS — $67,973 — 01-01
W. B. White - Materials Research Lab.

Structure and stability of insulator glasses with transition metal oxide additions; degree of order, structure of modifier and transition metal site; theory of crystal field effects and electronic transitions in glass environment; glass structure relative to crystals of same composition; phase separation; leaching; Raman 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.

UNIVERSITY OF PITTSBURGH

280. STUDIES FOR THE PRODUCTION OF SUPER-PURE SILICON NITRIDE — $37,000 — 03-03
P. E. D. Morgan - Dept. of Metallurgical and Materials Engineering

Synthesis of pure amorphous silicon nitride by three techniques: Iodine 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

281. CHEMICAL POISONING IN HETEROGENEOUSLY CATALYZED REACTIONS — $44,000 — 03-01
S. L. Bernasek - Dept. of Chemistry

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 heterogenously catalyzed reactions.

PURDUE UNIVERSITY

282. TRANSPORT AND THERMODYNAMIC PROPERTIES OF SOLIDS — $36,571 — 01-03
R. E. Grace - School of Materials Engineering

Chemical interdiffusion and interface stability in solid multicomponent, multiphase alloys; theory and experiment; kinetics and thermodynamics of interface instabilities; intrinsic and interdiffusion coefficients; electron microprobe and scanning electron microscopy; Cu-Ni-Zn, Fe-Ni-Al, and Fe-Ni-Cr alloy systems.

283. HIGH TEMPERATURE EFFECTS OF INTERNAL GAS PRESSURES IN CERAMICS — $56,205 — 01-03
A. A. Solomon - Dept. of Nuclear Engineering

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.

RENSSELAER POLYTECHNIC INSTITUTE

284. CHEMICAL DIFFUSION ON SOLID SURFACES — $33,800 — 01-03
J. B. Hudson - Dept. of Materials Engineering

Measurements of impurity diffusion on host surfaces-initially hydrogen, oxygen and sulfur on nickel; adsorption, desorption phenomena; techniques used: Auger electron spectroscopy, mass spectrometry.

RENSSELAER POLYTECHNIC INSTITUTE (CONTINUED)

285. THE EFFECT OF WELDING VARIABLES ON THE SOLIDIFICATION SUBSTRUCTURE, MECHANICAL PROPERTIES AND CORROSION BEHAVIOR OF AUSTENITIC STAINLESS STEEL WELD METAL — $49,000 — 01-01
W. F. Savage and D. J. Duquette
Materials Division

Corrosion behavior of stainless steels containing welds and stainless steel weldments; pitting and stress corrosion cracking in chloride containing solutions; potentio-dynamic and galvanokinetic test procedures; optical and electron metallography; stress corrosion cracking at slow strain rates in pressure vessels with electrochemical monitoring of potentials.

286. FATIGUE BEHAVIOR OF BCC METALS — $44,000 — 01-02
N. S. Stoloff - Dept. of Materials Engineering

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 temperature and above; V, Nb, V-H and Nb-H alloys.

UNIVERSITY OF ROCHESTER

287. THE MATERIALS AND MECHANICS OF RATE EFFECTS IN BRITTLE FRACTURE — $50,377 — 01-02
S. J. Burns - Dept. of Mechanical and Aerospace Sciences)

Experimental and analytical studies of crack growth dynamics in steel and brittle polymers; more precise techniques for measuring the critical stress intensity factor; ductile-brittle transitions in steel; crack velocities in double cantilever beam samples; critical comparison between new and conventional techniques for measuring crack velocities.

288. DIFFUSIONAL CREEP OF MULTI-COMPONENT SYSTEMS — $52,000 — 01-02
J. C. M. Li - Dept. of Mechanical and Aerospace Sciences

Impression creep testing as a convenient substitute for conventional creep testing using bulk specimens; studies of single crystals of beta-tin, Cu-Ni, Bi-Sb; diffusion mechanisms in amorphous alloys; constitutive equations.

UNIVERSITY OF SOUTHERN CALIFORNIA

289. ELECTRICAL AND MECHANICAL PROPERTIES OF OXIDE CERAMICS — $53,560 — 01-03
F. A. Kroger - Electronic Sciences Laboratory

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; polycrystalline Al_2O_3, pure and doped with Fe, Mg, Ti, or Si.

290. GRAIN BOUNDARY SLIDING DURING HIGH-TEMPERATURE CREEP — $75,000 — 01-02
T. G. Langdon - Dept. of Materials Science and Mechanical Engineering

Investigation of mechanisms controlling high temperature creep and rupture of metals (Al and Mg alloys) and ceramics (alkali halides, oxides); grain boundary sliding; dislocation glide and climb; cavity formation during creep.

291. EVAPORATION DRIVEN LIQUID SINTERING — $39,960 — 01-01
J. W. Whelan - Dept. of Materials Sciences

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

STANFORD RESEARCH INSTITUTE

292. CHEMISTRY OF ZIRCONIUM RELATED TO THE BEHAVIOR OF NUCLEAR REACTOR FUEL CLADDING — $134,950 — 03-03
D. Cubicciotti - Dept. of Chemistry

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

293. PHOTOVOLTAIC MATERIALS RESEARCH - II-VI HETEROJUNCTIONS AND Cu_2S/CdS THIN FILMS — $99,000 — 01-03
R. H. Bube - Dept. of Materials Sciences and Engineering

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; measurements of J-V curves in dark and light; junction capacitance; spectral response; diffusion lengths.

294. SUPERCONDUCTING AND SEMICONDUCTING PROPERTIES OF ELECTRON BEAM EVAPORATED MATERIALS — $75,000 — 02-02
T. H. Geballe and M. R. Beasley - W. W. Hansen Laboratories of Physics

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

295. MODELING OF DEFORMATION AND FRACTURE IN HIGH-TEMPERATURE STRUCTURAL MATERIALS — $72,000 — 01-02
A. K. Miller and O. D. Sherby - Dept. of Materials Sciences

Use of a computer aided constitutive equation for describing the entire range of phenomena included in non-elastic deformation; improvement of MATMOD equations through experimentation and analysis; study of kinematic hardening by using reversed torsion testing; transient hardening and softening effects; application of current MATMOD equations to the modeling of stainless steel and 2-phase nickel alloys.

296. STRUCTURE DEPENDENCE OF HIGH TEMPERATURE DEFORMATION OF METALS — $65,000 — 01-02
W. D. Nix - Dept. of Materials Science and Engineering

Determination of high temperature creep in metals; effects of grain size and shape in Ni, cavities in Ag, and impurity distribution on grain boundaries in Fe; analysis of cavity for motion and coalescence during creep.

STANFORD UNIVERSITY (CONTINUED)

297. DIFFUSION OF OXYGEN IN LIQUID METAL SYSTEMS — $46,000 — 01-03
D. A. Stevenson - Dept. of Materials Science

Oxygen solubility, thermodynamic activity and diffusion in liquid metal alloy solutions; calorimetric titration and time dependent currents using oxygen ion conducting solid electrolytes; aging of solid oxide 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

298. SURFACE CHARACTERIZATION OF CATALYTICALLY ACTIVE METAL ALLOY AND COMPOUND FILMS — $80,000 — 01-01
R. W. Vook - Chemical Engineering and Materials Science Department

Correlate structural, microstructural, and chemical parameters of thin epitaxial surface layers with their catalytic activities; oxidation of CO and surface catalytic activities determined from partial pressure measurements of CO, O_2 and CO_2; effects of ledges, strain, dislocations, crystal orientation, surface composition; Pt on Au or Cu; reflecting high energy electron diffraction, Auger electron spectroscopy, transmission electron microscopy.

UNIVERSITY OF TEXAS

299. SYNTHESIS OF NEW FUNCTIONALIZED FLUOROCARBON POLYMERS FOR USE AS BATTERY SEPARATORS AND MEMBRANES — $107,000 — 03-02
R. J. Lagow - Dept. of Chemistry

Synthesis of polymers by oxyfluorination to convert the terminal 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.

UNIVERSITY OF UTAH

300. POSITRON LIFETIME MEASUREMENTS AS A NONDESTRUCTIVE TECHNIQUE TO MONITOR FATIGUE DAMAGE — $53,746 — 01-02
J. G. Byrne - Dept. of Mechanical Engineering

Application of positron annihilation to the detection of early fatigue damage; correlation to electron microscopy, x-ray particle size and texture measurements; elastic fatigue in copper; fatigue hardening in steel; interaction of hydrogen with dislocations in nickel.

301. IMPURITY EFFECTS ON THE CREEP OF POLYCRYSTALLINE MAGNESIUM AND ALUMINUM OXIDES AT ELEVATED TEMPERATURES — $39,968 — 01-02
R. S. Gordon - Materials Science and Engineering Division

Determination of mechanisms of high temperature creep of polycrystalline oxide ceramics; 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.

302. ELECTROLYTIC DEGRADATION OF LITHIA-STABILIZED β"-ALUMINA — $64,000 — 03-02
D. K. Shetty and A. V. Virkar - Dept. of Materials Science and Engineering

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.

U. S. STEEL CORPORATION

303. STUDIES OF FUNDAMENTAL FACTORS CONTROLLING CATALYZATION OF REACTIONS OF GASES WITH CARBONACEOUS SOLIDS — $64,000 — 01-01
R. M. Fisher - Research Laboratory

Studies of the mechanism of graphite catalyzed with Fe particles; in-situ observations using high voltage electron microscopy; crystallographic observations coupled with reaction rate studies; role of impurities in graphite; quantitative measurements of the characteristics of reaction channels.

VARIAN ASSOCIATES

304. RESEARCH ON LATTICE MISMATCHED SEMICONDUCTOR LAYERS — $90,000 — 01-03
R. L. Bell - Solid State Laboratory

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; pn junction characteristics.

UNIVERSITY OF WISCONSIN

305. VOID NUCLEATION AND GROWTH IN HEAVY ION AND ELECTRON BOMBARDED PURE METALS — $72,828 — 01-04
G. L. Kulcinski - Dept. of Nuclear Engineering

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; electron microscopy and swelling; high voltage electron microscopy; 18 MeV copper bombardment of V; 1MeV electron bombardment of Al.

306. LOCAL ELECTRONIC PROPERTIES OF SEMICONDUCTOR SURFACES AND INTERFACES — $62,680 — 02-02
M. G. Lagally - Dept. of Metallurgical and Mineral Engineering

The local electronic properties of surfaces and interfaces of some elemental and compound semiconductors will be studied using Auger Electron Spectroscopy (AES). In addition chemisorption of Cl and O on Si will be studied AES will be augmented with XPS and UPS to investigate a series of orthohombic IV-VI semiconductor compounds.

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, 1977, the Materials Sciences total support level amounted to about $52.8 million in operating funds and $5.1 million in equipment funds. The equipment funds are expended primarily at ERDA 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.)	43.1	16.9
(b) South ..... (Fla., N.C., Tenn., Va., Georgia)	4.1	24.2
(c) Midwest ..... (Ohio, Ill., Wisc., Mich., Minn., Ind., Iowa, Kan.)	18.3	38.7
(d) West ..... (Ariz., Okla., Wash., Texas, Hawaii, N.Mex., Calif., Utah, Col., Idaho)	34.5	20.2
	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-)	62.1	43.5

	Contract Research (%)	Total Program (%)
(b) Physics, Solid State Science, Solid State Physics (Office Budget Activity Numbers 02-)	29.7	41.1
(c) Chemistry, Chemical Eng. (Office Budget Activity Numbers 03-)	8.2	15.4
	100.0	100.0

3. By ERDA 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)	35.8
(b) Laboratory Program	64.2
	100.0

4. By Laboratory:

	Total Program (%)
Ames Laboratory	9.7
Argonne National Laboratory	22.7
Brookhaven National Laboratory	10.6
Idaho National Engineering Laboratory	.3
Illinois, University of (Materials Research Laboratory)	3.1
Lawrence Berkeley Laboratory	8.2
Lawrence Livermore Laboratory	1.5
Los Alamos Scientific Laboratory	1.7
Mound Laboratory	.4
Oak Ridge National Laboratory	23.5
Pacific Northwest Laboratory	2.2
Sandia Laboratory	1.3
Contract Research	14.8
	100.0

5. By Selected Areas of Research:

	Number of Projects (Total=301) (%)	Total Program $ (%)
(a) Materials		
Actinide Metals and Compounds	6.7	3.6
BCC Refractory Metals	17.0	7.4
Ceramics	25.6	14.4
Rare Earth Metals and Compounds	8.7	4.3
Liquids	9.3	5.9
Semiconductors	11.3	5.9
(b) Technique		
Neutron Scattering	7.0	15.0
Theory	14.0	8.7
(c) Phenomena		
Catalysis	6.0	4.1
Corrosion & Stress Corrosion Cracking	7.0	3.4
Diffusion	10.6	4.5
Superconductivity	8.0	8.6
Strength	18.6	10.9
Surface Phenomena & Thin Films	13.3	10.1
(d) Environment		
Hydrogen	10.0	4.6
Radiation	11.3	16.2

SECTION D

Index of Investigators, Materials, Phenomena, Technique and Environment

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

Abraham, M. M., 165, 167, 169
Ackermann, R. J., 66
Agrawal, A. K., 274
Aldred, A. T., 36, 37
Alkire, R. C., 92
Allen, C. W., 271
Allred, D. D., 175
Altstetter, C. J., 97
Anderson, A. C., 103
Anderson, J. L., 149
Anderson, M. S., 22
Appleton, B. R., 166, 169, 171, 175, 176
Arai, T., 61
Arbel, A., 76
Ardell, A. J., 204
Argon, A. S., 254
Arko, A. J., 40
Arsenault, R. J., 252
Ast, D. G., 229
Atoji, M., 63
Aubry, S., 85
Averback, R. S., 48
Axe, J. D., 78, 79, 80

Bacarella, A. L., 181
Bader, S. D., 38
Baikerikar, K. G., 35
Bailey, D. M., 16
Balluffi, R. W., 230
Barnes, R. G., 20
Barrett, J. H., 172
Bates, J. B., 165, 169
Bates, J. K., 64
Battle, G. C., 167
Bautista, R. G., 30, 32
Beasley, M. R., 294
Beatty, R. L., 151
Beaudry, B. J., 3
Begun, G. M., 178
Bell, J. T., 178
Bell, R. L., 304
Benedek, R., 48
Bennett, B. I., 147
Bennett, S. L., 151
Benson, J. E., 27
Bentley, J., 160
Berard, M. F., 10
Berger, A. S., 45
Bernasek, S. L., 281
Bevolo, A. J., 22
Bilello, J. C., 264
Billington, D. S., 160
Birnbaum, H. K., 96
Birtcher, R. C., 47
Blakely, J. F., 38
Blander, M., 68, 71, 72, 74
Blewitt, T. H., 47
Blum, L., 177
Blume, M., 85
Bonilla, C. F., 225
Borie, B. S., 155
Bowen, H. K., 255
Bragg, R., 124
Brandt, E. H., 25
Braski, D. N., 154
Braunstein, J., 179, 180
Brewer, L., 133
Brimhall, J. L., 188
Brodsky, M. B., 38, 40
Broutman, L. J., 249
Brower, K. L., 192
Brown, B. S., 47
Brown, G. M., 177
Brown, R. D., 146
Brun, T., 50
Brundage, W. E., 167
Bube, R. H., 293
Burkhart, L. E., 33
Burnet, G., 30, 31
Burns, S. J., 287
Busch, R., 190
Busing, W. R., 177
Butler, M. A., 194
Butler, W. H., 152
Byrne, J. G., 300

Cable, J. W., 163
Cafasso, F. A., 73
Calaway, W., 67
Cappelletti, R. L., 162
Carlson, O. N., 1, 4
Carlson, P. T., 157

Carlson, R. D., 155
Carpenter, J. M., 51
Carpenter, R. W., 156, 160
Cartens, D. H. W., 149
Cathcart, J. V., 157
Caton, R., 76
Chang, S. J., 170
Chang, Y. K., 167
Charlot, L. A., 188
Chen, C. W., 11, 17
Chen, H., 43
Chen, W. K., 44, 45
Chen, Y., 165, 167
Chikalla, T. D., 182
Child, H. R., 163, 164
Chiotti, P., 16
Christen, D. K., 163, 166
Clark, G. J., 171, 175
Clark, G. W., 153
Clarke, J., 128
Cleland, J. W., 167, 169
Clem, J. R., 25
Cline, C., 140, 141
Coble, R. L., 258
Coghlan, W. A., 160
Cohen, M., 129
Coltman, R. R., 173
Connolly, T. F., 167
Cooke, J. F., 172
Cooper, A. R., 214
Corbett, J. D., 28
Cowley, J. M., 202
Cox, D. E., 88
Crabtree, G., 56, 57
Crawford, R., 50
Crummett, W. P., 162
Cubicciotti, D., 292
Curtiss, L., 72

Dahlgren, S. D., 183, 185
Danielson, G. C., 22
DasGupta, A., 159
David, L., 163
Davis, H. L., 172
Davis, M., 191
DeJonghe, L. C., 231
Delbecq, C., 53, 60
Devereux, O. F., 226
Dew-Hughes, D., 76
Dickmann, J. E., 87
Dienes, G. J., 85
DiMelfi, R. J., 49
Doll, J. D., 266
Donaghey, L. F., 135
Dow, J., 104
Drickamer, H. F., 105
Dunlap, B., 57
Duquette, D. J., 285
Duwez, P., 210
Dye, D. H., 57

Early, B. F., 169
Easton, D. S., 159
Eckels, D. E., 22
Eckert, J., 79, 80, 81
Edelstein, A. S., 18
Ellenson, W. D., 79, 80, 81
Emery, V. J., 85
Engstrom, H., 84, 87
Engstrom, H. L., 165

Faber, J., 44
Falco, C., 55, 56
Farrell, K., 160
Faulkner, J. S., 152
Fekbelman, P. J., 193
Felcher, G., 50, 56
Feldman, R. D., 166
Finch, C. B., 153
Finnemore, D. K., 23
Fisher, E. S., 45
Fisher, R. M., 303
Flotow, H. E., 63, 65
Fluss, M. J., 45
Follstaedt, D. M., 192
Fradin, F. Y., 36, 43
Franzen, H. F., 34
Fraser, H. L., 95
Frazer, B. C., 84, 88
Freyhardt, H. C., 159
Fuchs, R., 26
Fulrath, R., 123
Furrer, M., 179
Furtak, T. E., 21

Galligan, J. M., 227
Geballe, T. H., 294
Gerstein, B. C., 35
Ghosh, A., 82
Gibala, R., 215
Gilbert, T. L., 60, 61
Ginley, D. S., 194
Ginsberg, D. M., 107
Girard, C. A., 179, 180
Godgrey, T. G., 158
Goland, A. N., 86, 87, 89
Goldman, A. M., 262
Goldstone, J., 146
Gole, J. L., 256
Goodwin, G. M., 161
Gordon, R. L., 189
Gordon, R. S., 301
Grace, R. E., 282
Granato, A. V., 106
Grant, N. J., 257
Gray, K., 55
Green, W. V., 146
Gruen, D. M., 64
Gschneidner, K. A., 3, 11, 13
Gupta, R. P., 45
Gurinsky, D. H., 76
Gurland, J., 203
Guttman, L., 59
Gyorffy, B., 152

Habenschuss, A., 21
Hafstrom, J., 55
Halevi, P., 26
Hansen, R. S., 35
Hariharan, A. V., 34
Harmon, B. N., 24
Harris, L. A., 151
Hart, E. W., 234
Hartley, C. S., 242
Hartman, J. S., 189
Hastings, J. M., 84
Hays, D. D., 190
Hecker, S. S., 145
Heldt, L. A., 261
Helland, B. J., 27
Henager, C. H., Jr., 183, 185
Hendrick, P. L., 188
Hendricks, R. W., 155
Herbst, J. F., 85
Herley, P. J., 265
Heuer, A. H., 216
Hinks, D. G., 52, 60
Hoke, J. H., 277
Holder, J. D., 153
Holmes, D. K., 172
Holt, B., 69
Hoover, W. R., 195
Hopper, R., 140
Houston, J. E., 193
Howng, W. Y., 66
Hren, J. J., 242
Hsiang, T. Y., 23
Hubbard, W. N., 70
Hubble, B., 69
Hudson, J. B., 284
Hunter, O., 5
Hwang, Y. S., 20

Imoto, H., 28
Isaacson, H. R., 69
Iton, L., 56
Iwata, T., 176

Jaccarino, V., 209
Jackson, J. J., 60, 62
Jacobson, R. A., 27
Jager, W. B., 48
Jeffries, C., 127
Jenkins, L. H., 168
Johnson, C. E., 70
Johnson, C. K., 177
Johnson, G. K., 70
Johnson, H. H., 232
Johnson, P. L., 63
Johnson, S., 69
Joiner, W. C. H., 220
Jonas, J., 93
Jones, R. H., 184
Jones, R. O., 152
Jorgensen, J. D., 50, 60
Jung, P., 160
Jura, G., 131

Kamitakahara, W. A., 18
Kammerer, O., 76
Kaneda, T., 165
Kaplan, T., 172
Karim, D., 37
Kayser, F. X., 15
Keiser, D. D., 90, 91
Kelly, E. J., 181
Kendig, M. W., 75
Kenik, E. A., 160
Kerchner, H. R., 166
Kerley, G. I., 147
Kernohan, R. H., 166
Key, J. F., 90
Khan, J., 143
Khatamian, J., 18
Khattak, C., 88
Kierstead, H. A., 54, 57
Kim, K. K., 44, 45, 70
Kingery, W. D., 258
Kirk, N. A., 47
Kirk, W., 148
Kissinger, H. E., 188
Klabunde, C. E., 173
Kleb, R. K., 50, 51
Klemm, R. A., 25
Kliewer, K. L., 26
Kline, G. R., 18
Knapp, G. S., 43
Knotek, M. L., 194
Koch, C. C., 159
Kocks, J. F., 42
Koehler, J. S., 112
Koehler, W. C., 162, 163, 164
Koelling, D., 61
Kohlstedt, D. L., 233
Kopp, O. C., 153
Kosel, T. H., 41
Krauss, A. R., 64
Krefft, G. B., 192
Krikorian, O., 139
Krinsky, S., 85
Kroeger, D. M., 159
Kroger, F. A., 289
Kuczynski, G. C., 271
Kulcinski, G. L., 305
Kumar, R., 69
Kunitomi, N., 162
Laegreid, N., 190
Lagally, M. G., 306
Lagow, R. J., 299
Lam, D. J., 36, 37
Lam, N. Q., 45, 46
Lance, R. H., 234
Lander, G. H., 39
Landman, U., 244
Langdon, T. G., 290
Langford, G., 239
Larson, B. C., 169, 174
Lau, K., 61
Lawrence, W. E., 240
Lax, M., 263
Lazarus, D., 108
Lee, K., 76
Lefakis, H., 47
Legvold, S., 19
Leitnaker, J. M., 154
Lessor, D. L., 189
Levinson, L. S., 146
Levy, A., 119
Levy, H. A., 177
Levy, P. W., 86, 87
Lewis, M. B., 160
Li, C.-Y., 235
Li, J. C. M., 288
Lin, J., 155
Liu, M. B., 64
Liu, S. H., 24
Livesay, B. R., 245
Loomis, B. A., 47
Lumwalt, L., 267
Lundy, T. S., 157
Lutz, H., 82
Lyles, R. L. Jr., 48
Lynch, D. W., 21
Lynn, K. G., 86, 87

Machida, K., 25
Maglic, R., 50
Mahoney, J. V., 303
Manghnani, M. H., 246
Mansur, L. K., 160
Maple, M. B., 207
Marcinkowski, M. J., 253

Maroni, W. A., 67
Marshall, S., 53, 60
Martinoli, P. S., 23
Matlock, D. K., 224
Matson, M. S., 29
McBeth, R. L., 64
McCarley, R. E., 29
McClintock, F. A., 254
McCreary, J. R., 66
McElroy, D. L., 158
McKee, R. A., 157
McMasters, O. D., 11
McMillan, J. A., 59
Meckling, H., 42
Melendres, C., 71, 73
Melius, C. F., 195
Mendelsohn, M. H., 64
Merkle, K. L., 48
Merz, M. D., 186, 187
Meshii, M., 269
Metzger, M., 94
Michels, D. E., 91
Milam, D., 142
Miller, A. K., 295
Miller, D. L., 82
Miller, J. F., 45
Mills, R. L., 148
Mitchell, T. E., 217
Miwa, H., 162
Miyano, J., 58
Mockler, R., 222
Modine, F. A., 165
Moehlecke, S., 77
Montroll, E. W., 244
Mook, H. A., 162, 164
Moon, R. M., 163
Moore, J. P., 158
Morgan, P. E. D., 280
Morosin, B., 194
Morral, J. E., 228
Morris, J. W., 116
Moss, S. C., 248
Mostoller, M. E., 172
Moteff, J., 221
Mueller, B. A., 145
Mueller, F., 61
Mueller, M. H., 39
Mulford, R. A., 42
Muller, R. H., 136
Mundy, J. N., 45
Murch, G. E., 66
Murphree, Q. C., 175
Murtha, M. J., 31
Myers, S. M., 192

Nagy, Z., 71, 74
Narayan, J., 170, 174, 176
Narten, A. H., 177
Nelson, R. D., 186
Nicklow, R. M., 162, 163, 164
Nix, W. D., 296
Noer, R. E., 23
Noggle, T. S., 168, 170, 174, 176
Nolfi, F. V., 49
Noonan, J. R., 168
Norris, C. B., 192
Notis, M., 251

Oen, O. S., 172, 176
Ogle, J. C., 156
Ohr, S. M., 170, 174
Okamoto, P. R., 49
Olander, D., 134
Olsen, L. C., 182
Olson, C. G., 21
Olson, D. L., 224
O'Reilly, D., 56
Orent, T. W., 35, 38
Osborne, D. W., 65
Osmun, J. W., 23
Ostenson, J. E., 23
O'Sullivan, W., 222

Packan, N. H., 160
Painter, G. S., 152
Palko, A. A., 181
Pande, C., 76
Panitz, J. A., 193
Papatheodorou, G., 68
Parker, E., 117
Parkin, D. M., 146
Parra, R., 163
Pask, J. A., 121
Passell, L., 78, 80, 81
Patterson, J. W., 11
Pawel, R. E., 157

Pawlewicz, W. T., 183, 190
Payne, D. A., 102
Peercy, P. S., 192
Pelizzari, C., 50
Perkins, R. A., 157
Petersen, G. F., 157
Peterson, D. T., 7, 8
Peterson, N. L., 44
Peterson, S. W., 63
Phillips, N. E., 130
Phoenix, S. L., 236
Pick, M., 76
Pickus, M., 115, 120
Picraux, S. T., 192
Pigg, J. C., 165
Pines, A., 138
Pipes, P. B., 241
Polgreen, T. L., 169
Pong, W., 247
Posey, F. A., 181
Postol, T., 50
Potter, D. I., 49
Primak, W., 60, 62
Pronko, P. P., 48
Pugh, E. N., 99
Pyper, P., 144

Rahman, A., 61
Raj, R., 237
Rapp, R. A., 272
Rauh, E. G., 66
Rechtin, M. D., 44, 49
Redman, J. D., 178
Redman, J. K., 173
Reed-Hill, R. E., 243
Rehn, L. E., 49
Reiley, T. C., 160
Reis, A. H., 63
Reyes, J., 26
Ricci, E., 155
Rice, J. R., 203
Richards, P. L., 125
Rimbey, P. R., 26
Roach, P. R., 54, 58
Roberto, J. B., 174
Robinson, C. C., 167
Robinson, J., 61
Robinson, M. T., 172
Rosei, R., 21
Rosner, J. S., 89
Rothman, S. J., 45, 46
Routbort, J. L., 42
Rowland, T. J., 101
Rye, R. R., 193

Saboungi, M., 68, 71, 74
Sagues, A. A., 49
Sari, S., 201
Savage, W. F., 285
Scattergood, R. O., 41, 42
Schirber, J. E., 194
Schmidt, F. A., 1, 2
Schow, O. E.,
Schultz, A. J., 63
Schwarz, R., 42
Scott, T. E., 6, 9
Searcy, A., 122
Seidman, D. N., 238
Sekerka, R. F., 213
Sekula, S. T., 166
Selman, J. R., 250
Shanks, H. R., 22
Shapiro, S. M., 78, 79, 80, 81
Sheldon, R., 66
Shen, Y., 126
Shenoy, G., 57
Sherby, O. D., 295
Sherrill, F. A., 174
Sherry, E. G., 63
Shetty, D. K., 302
Shewmon, P. G., 273
Shirane, G., 78, 79, 80
Short, D. W., 139
Shull, C. G., 259
Sickafus, K., 168
Siegel, R. W., 45, 46
Siegel, S., 73
Simanek, E., 206
Simmons, M. L., 146
Simmons, R. O., 109
Simonen, E. P., 188
Sinha, S. K., 50
Skold, K., 50
Slichter, C. P., 110
Smedskjaer, L. C., 45
Smith, D. Y., 59
Smith, F. J., 178
Smith, H. G., 162, 164, 166
Smith, J. F., 11, 12, 16

Smyrl, W. H., 191
Snead, C. L., 77
Sokoloff, J., 268
Solin, S. A., 219
Solomon, A. A., 283
Sommer, W. F., 146
Somorjai, G., 137
Sonder, E., 165
Souers, C., 144
Sparks, C. J., 155
Spedding, F. H., 21
Spooner, S., 164
Staehle, R. W., 274
Stapleton, H. J., 165
Stark, W. A., 149
Stassis, C., 18
Stein, D. F., 261
Stevenson, D. A., 297
Stiegler, J. O., 160
Stocks, G. M., 152
Stoloff, N. S., 286
Storms, E. K., 145
Strongin, M., 82, 83, 89
Strozier, J., 83
Suenaga, M., 76
Summers, G. P., 275
Susman, S., 52, 60
Swansiger, W. A., 195
Swendsen, R. H., 85
Swenson, C. A., 22
Swyler, K. J., 86

Tam, S. W., 45
Tarvin, J. A., 78, 81
Taylor, A., 49
Thiessen, W. E., 177
Thomas, G., 113
Thomas, G. J., 195
Thomas, M. T., 184
Thomlinson, W. C., 78, 80, 81
Thorel, P., 164, 166
Thorn, R. J., 66
Thrower, P. A., 278
Tobias, C. W., 132
Tohver, H. T., 165
Torgeson, D. R., 20
Trivedi, R. K., 2, 4
Troiano, A. R., 218
Tschoegl, N. W., 211
Tsunoda, Y., 162
Tuller, H. L., 260
Turcotte, R. P., 182
Turner, A. P. L., 41, 42

Ulehla, M., 172

Vallet, C. E., 179, 180
Vandermeer, R. A., 156
Vashishta, P., 61
Vaughan, R. W., 212
Veal, B. W., 36, 37
Veleckis, E., 67
Verhoeven, J. D., 11, 13, 14
Virkar, A. V., 302
Vogel, G., 176
Vook, F. L., 192, 193
Vook, R. W., 298
Vyas, B., 75

Wakabayashi, N., 162, 164
Wang, J. C., 165
Wang, R., 183, 185
Washburn, J., 118
Watson, R. E., 85
Weaver, J. H., 21
Webb, R., 54, 56
Weber, M., 141, 142
Wechsler, M. S., 17
Weeks, J. R., 75
Weeks, R. A., 165
Welch, D. O., 76, 85
Wendelken, J. F., 168
Wert, C. A., 98
Westbrook, R. D., 167, 169
Westerman, R. E., 184
Westlake, D. G., 45
Westmacott, K., 114
Weyhmann, W. V., 262
Wheatley, J. C., 208
Whelan, J. W., 291
White, C. L., 156
White, C. W., 171, 175
White, W. B., 279
Whitmore, D. H., 270
Whitten, J. L., 266

Wiedersich, H., 49
Wilder, D. R., 10
Willemsen, H., 55
Williams, D. E., 2
Williams, J. M., 173, 176
Williams, R. K., 158
Williams, W. S., 111
Wilson, W. D., 195
Winslow, G. H., 66
Wirtz, G. P., 100
Wolf, E. L., 23
Wood, C., 165
Wood, R. F., 169, 172
Worrell, W. L., 276
Wright, R. B., 64
Wu, C., 55
Wuensch, B. J., 255

Yakel, H. L., 155
Yarlagadda, B., 61
Yen, C. F., 153
Yonco, R. M., 67
Yoo, M. H., 152
Young, R. T., 169
Yu, M., 83
Yue, A. S., 205
Yust, C. S., 151
Yuster, P., 53, 60

Zackay, V., 117
Zaitlin, M., 23
Zehner, D. M., 168
Zimmermann, W., 262
Ziomek, J., 66

Actinide Metals and Compounds

1	66
11	70
17	134
18	151
36	156
39	158
40	164
57	172
63	186
65	255

Ceramics

Carbides

62	187	
65	228	
66	233	
95	256	
98	291	
111		
151		
154		
172		

Glass

36	142	
86	182	
121	192	
141	214	
	219	
	279	

Nitrides

62	237	
65	250	
66	280	
70		

Oxides

5	98	178
10	100	182
22	102	190
31	103	192
37	113	194
39	119	216
41	121	217
42	122	231
44	123	251
52	141	255
60	143	258
62	155	260
65	157	275
66	158	277
69	162	283
84	163	289
86	165	290
87	167	291
88	172	301
91	175	302

Composites

13	153
14	157
23	205
76	213
94	236
120	249
124	254
151	304

Fast Ion Conductors

44	164
51	165
61	209
71	212
81	260
85	270
103	272
108	276
157	297
	302

Graphite, Carbon, and Coal

27	155
35	177
63	250
80	267
81	278
124	303
138	
151	

Hydrides

6	63	212
20	64	232
39	76	245
50	96	248
51	98	265
57	164	286

Intermetallic Compounds

11	23	76	159
13	24	77	166
15	38	82	167
18	43	88	185
20	52	89	207
21	55	115	253
22	57	120	294

Ionic Crystals

22	52	86	164
24	53	91	179
27	68	122	247
28	69	141	270
34	71	142	272
50	84	145	290

Liquids & Amorphous Metals

21	58	78	132	177	250
26	59	82	138	179	288
30	67	118	140	180	297
32	68	125	147	191	
33	72	126	150	210	
50	74	130	162	222	

Metals

Alkali

16				
65				
67				
149				
178				
224				
225				
276				
302				

BCC Refractory

1	29	149	174	238
3	34	156	175	241
4	45	157	188	243
6	67	159	195	246
7	77	160	215	248
8	97	164	217	252
12	98	166	221	264
17	128	167	227	269
20	139	171	228	281
23	146	173	232	286
				305

Ferrous

4	113	163	210	261
6	115	164	217	269
9	116	167	218	273
16	117	173	224	274
42	119	174	226	282
47	139	181	232	285
67	154	184	235	287
75	157	187	238	295
76	158	191	239	296
91	160	192	254	303
92	162	195	257	
		203		

MHD Materials

10	65	
37	66	
44	88	
60	153	
62		

Polymers

22	141	
63	155	
70	177	
72	193	
93	211	
101	236	
105	247	
109	249	
	299	

Rare Earth Metals and Compounds

1	19	50	115	210
3	21	52	149	245
11	24	57	151	
13	28	63	162	
15	30	65	163	
18	39	70	172	

Semiconductors

2	110	175
3	118	182
21	125	183
22	126	192
26	127	201
35	129	205
52	130	229
59	153	247
61	167	258
82	169	293
104	171	304
		306

Acoustic Emission

91
99

Auger Electron Spectroscopy

35 230
38 245
91 261
168 284
182 298
224

Computer Simulation

61
66
85
116
174
180

Elastic Constants

5
12
106
211
246

Electron Microscopy

9	73	151	202	230	257
17	75	160	204	231	258
41	95	170	215	233	264
42	113	174	216	242	271
45	114	187	217	243	298
48	118	188	221	245	303
49	123	190	224	251	305
69	145	195	229	253	

Electron Spin Resonance

53
56
60
165
169
209

Field Emission and Ion Microscopy

35
193
238

High Temperature Heat Capacity

30
158

Infrared Spectroscopy

21 150
69 165
125 219
144

Internal Friction

42
96
106
243

Ion Channeling, Scattering and Implantation

48 137
49 169
56 171
64 175
87 192
89 250
118 255
134

Laser Beam Scattering

64
126
142
143
189
219
222

Low Temperature Specific Heat

40
43
54
65
76
130
158
159

Magnetic Susceptibility

11
19
36
37
40
54
57
210
245
262

Neutron Scattering

18
27
39
44
50
51
63
76
78
79
80
81
84
88
162
163
164
166
169
177
259

Nuclear Magnetic Resonance

20
35
36
54
56
101
110
138
209
212
270

Optical Spectroscopy

21
26
32
58
59
126
136
141
165
189
190
201
222
247
258
275
279

Positron Annihilation

45
77
86
87
248

Sputtering

22
23
64
97
183
185
187
238

Synchrotron Radiation

21
84
104
155

Theory

2	61	152	214	266
16	66	160	228	268
24	68	172	234	273
25	71	174	235	288
26	85	194	236	291
42	116	195	240	295
48	129	203	244	
49	133	206	249	
59	147	213	263	

Thermal Conductivity

5
10
22
60
72
158

Thermodynamics

1	139
7	144
22	145
65	149
66	154
68	157
70	158
72	178
73	179
121	211
122	225
131	226
132	272
133	292

X-Ray Photoelectron Spectroscopy

36
38
43
63
66
306

X-Ray Scattering

15	91
27	124
34	140
39	145
42	155
63	174
66	190
69	219
73	229
75	246
76	248
84	250
88	

Catalysis

26 100 298
29 110 303
35 111
38 152
56 168
61 177
68 223
83 281

Channeling

48
87
89
175

Corrosion

15 187
16 224
21 226
91 274
92
139
181

Crystal Structure, Atomic Distribution and Crystal Transformations

4 68 140
16 69 144
20 79 154
27 93 177
34 95 211
50 109 219
63 113 246
279

Diffusion

1 96 249
4 108 255
7 109 272
10 121 273
20 157 282
33 178 284
44 180 288
45 192 297
46 195
50 214
66 216
67 230

Dislocations

118 233
152 242
174 253
216 268
226 269
230

Erosion

41
92
117
119
151

Electron and Ion Conduction

11 179
21 201
22 209
24 229
57 240
60 241
71 247
118 258
124 260
132 270
136 276
152 289
165 302

Electronic Structure

18 61 126
24 66 127
36 85 129
37 105 212
40 125 275

Magnetism

11 61 245
19 78 259
37 85 262
39 163
40 172
50 208
57 210

Materials Preparation and Characterization

2 31 167
3 52 205
8 60 280
11 88 299
14 102 304
28 140
30 153

Nondestructive Evaluation

12
300

Phonons

18 103
39 109
50 158
58 162
72 164
79 172
80 248
263

Photovoltaic and Photothermal Phenomena

2 150 229
3 152 293
21 153 304
22 168 306
26 171
32 182
59 183
110 194
111 201
118 205
129

Point Defects

17 106 204
45 112 217
47 114 221
48 160 238
49 165 248
53 173 252
62 176 269
77 182 275
84 188 305
86 192

Precipitation

4 113 283
47 155 305
49 160
74 204
95 228
97 271
98 273

Recovery and Recrystallization

17 118
47 143
48 173
49

Sintering

5 258
102 271
115 283
121 291
123
251

Solidification

14
147
213
214
257

Strength

Fracture

5 156 264
6 170 277
10 203 287
75 232
76 237
99 254
151 261

Constitutive Equations

41
234
235
288
295

Fatigue

42
184
249
286
300

Creep

42 257
160 258
188 288
221 290
233 296
251 301
254

Flow Stress

4 203 269
17 215 278
42 216
76 227
94 233
97 235
98 236
116 239
117 243
145 252
156 253
195 264

Stress-Corrosion Cracking

9 191
75 218
92 261
99 274
134 285
181 292
184

Superconductivity

13 120 262
23 128 294
25 159
43 164
50 166
55 172
61 185
76 207
78 210
82 220
107 227

Surface Phenomena and Thin Films

15 88 193 306
21 126 201
22 136 202
23 137 222
26 141 242
38 142 244
48 143 247
56 157 250
59 168 266
64 178 267
73 189 284
81 190 292
83 192 298

Welding

90
161
285

Gas

Oxidizing	Hydrogen			Sulphur-Containing
1	6	164	252	3
15	7	177	265	69
97	45	178	266	157
157	49	194	273	276
187	63	195	278	281
215	76	212	284	284
278	96	215	285	293
284	99	223	300	
297	107	232		
298	144	245		
306	149	248		

Magnetic Field

11	120
19	163
24	259
40	262
50	
57	

Pressure
Above Atmospheric

50
80
93
105
131
148
207
211
246
251

Radiation

Electron	Ion		Neutron		Photons	Theory	Gamma
48	47	165	17	176	104	49	53
86	48	171	47	188	142	160	87
112	49	174	77	221	189	172	165
114	62	175	86	252		188	223
134	64	176	160				
160	77	188	173				
269	86	204	174				
305	89	238					
	118	305					
	160						

Temperature

Very Low Temperatures

54
65
103
130
208
262

High Temperatures

30	146
32	153
34	154
60	158
66	225
72	254
119	255
122	256
124	295
133	296
134	
139	
145	