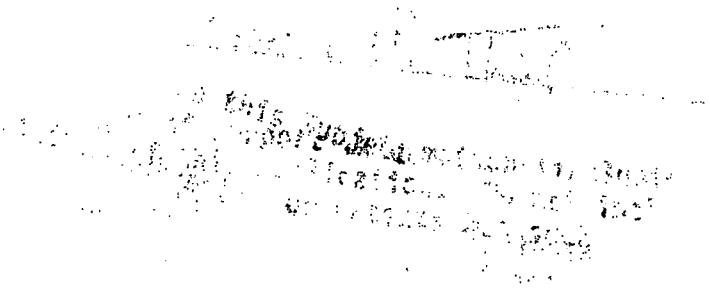
ERDA-76/123

Materials Sciences Programs

FY 1976

Energy Research and Development Administration

Division of Physical Research



ERDA-76/123
UC-25

Materials Sciences Programs

FY 1976

Energy Research and Development Administration

Division of Physical Research

FOREWORD

During FY 1976, a number of organizational changes took place within the Energy Research and Development Administration. The accompanying chart shows the ERDA organization as of July 1, 1976 and the location of the Physical Research Division. Six activities exist under the ERDA Administrator, each headed by an Assistant Administrator: National Security, Fossil Energy, Nuclear Energy, Conservation, Environment and Safety, and Solar, Geothermal, and Advanced Energy Systems. While organizationally the Division of Physical Research is located under the Assistant Administrator for Solar, Geothermal and Advanced Energy Systems, the mission of the Division is to provide the physical research base for all ERDA activities.

The Materials Sciences Subprogram constitutes one portion of a wide range of research supported by the ERDA Division of Physical Research. Other programs are administered by the Division's Nuclear Sciences, Molecular Mathematical and Geoscience Sciences, and High Energy Physics 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 underway in FY 1976 together with a convenient index to the program.

Donald K. Stevens
Assistant Director
(for Materials Sciences Program)
Division of Physical Research

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

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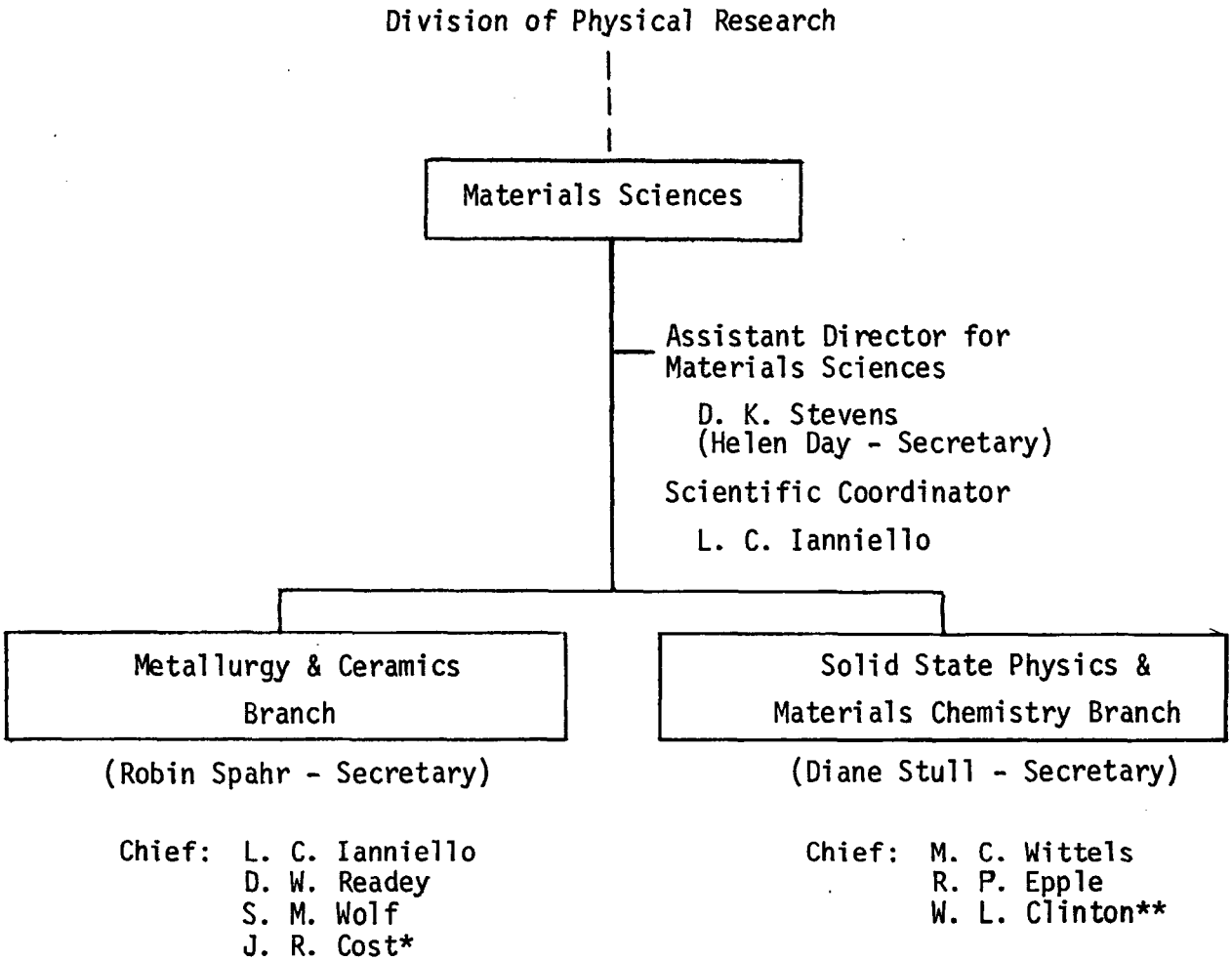
JULY 4, 1975

STRUCTURE OF MATERIALS SCIENCES SUBPROGRAM



* On Year's Leave from Purdue University - Starting 9/76
** On Year's Leave from Georgetown University - Starting 10/76

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SECTION A

Laboratories

The information was taken from current Laboratory program budget submissions. Most projects are of a continuing nature although specific problems and some projects were concluded in FY 1976.

AMES LABORATORY
Iowa State University
Ames, Iowa 50010

Metallurgy and Ceramics -01-
K. A. Gschneidner, Jr. - Phone: (FTS) 865-2272 or 515 294-2272

1. STRUCTURE OF MATERIALS $230,000 01-01
O. N. Carlson, F. A. Schmidt
R. K. Trivedi

The study of electrotransport and thermotransport properties of interstitial solutes (O, N and C) in refractory metals; mechanical studies of vanadium and other refractory metals; investigation of the properties and energy system applications of chromium-molybdenum ferritic steels; basic and theoretical studies of phase formation and properties of surfaces including the reactions of refractory metal surfaces to hydrogen environment; basic studies involving microstructural reactions at high temperatures; development of methods for the preparation of ultra pure metals, alloys and compounds in poly-and single-crystalline form with emphasis on rare earth (Sc and La) and refractory metals (V, Th, Nb, Ta and Ti); study of the effects of trace impurities and controlled alloy additions on the physical properties of materials; application of transport phenomena (electrotransport and the thermotransport) to metal purification.

2. MECHANICAL PROPERTIES $360,000 01-02
T. E. Scott, O. Hunter
D. T. Peterson

Studies of fabrication and basic mechanical behavior of refractory oxides (Y_2O_3, HfO_2, ZrO_2, MgO, etc.) and of the hydrogen attack of structural steels that are pertinent to fossil fuel utilization schemes such as MHD and coal gasification; investigation of hydrogen embrittlement of refractory metals (V, Nb, and Ta) and ferrous metals and the identification of mechanisms responsible for degradation of mechanical properties; relationship between stress conditions and hydrogen attack in ferrous materials will be studied; the stress induced relationships of refractory metal hydrides will be explored and the diffusion coefficients of hydrogen and deuterium in V and Nb will be measured.

AMES LABORATORY
Metallurgy and Ceramics -01- (Continued)

3. PHYSICAL PROPERTIES $700,000 01-03
J. F. Smith, D. M. Bailey,
M. F. Berard, C. W. Chen,
P. Chiotti, K. A. Gschneidner, Jr.,
F. X. Kayser, O. D. McMasters,
J. W. Patterson, J. D. Verhoeven,
D. R. Wilder, D. E. Williams

Thermodynamic and phase studies of fused salt and liquid metal systems pertinent to fossil fuel technology especially coal gasification, liquifaction and desulphurization; study and development of materials with optical and physical properties that enhance their utilization in solar devices - MgF_2 and complex rare-earth oxides are examples of materials being considered; work concerning the application of ceramics, aligned composite materials, and metals to the areas of energy storage, conversion and transmission; basic research relationships between the microstructures of materials and their electrical and mechanical properties; interdiffusion studies of ceramic systems, EMF measurements of new cell materials, preparation of aligned composites by directional solidification, and basic thermodynamic measurements are currently underway; development of refractory oxides and carbides for use as thermal and electrical insulators; study and control of reactions at metal - ceramic interfaces; physical, thermal and magnetic properties studies of rare-earth alloy systems; characterization of the allotropes of cerium; general and fundamental work on phase transformations; elastic constant determinations of superconducting materials.

4. RADIATION EFFECTS
M. S. Wechsler, C. W. Chen $310,000 01-04

Study of radiation induced changes in physical and mechanical properties of refractory metals; effects of trace impurities and alloy additions on radiation hardening and embrittlement; investigation and development of mechanisms to suppress void formation; the dopant effect on the suppression of void formation in doped V-Ti alloys will be studied; TEM studies of dislocation morphologies in irradiated niobium; the effects of microstructural factors, trace impurities, and radiation produced defects, on mechanical properties of FCC metals will be studied using thorium containing carbon.

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

5. NEUTRON SCATTERING $540,000 02-01
C. Stassis, W. A. Kamitakahara,
J. G. Traylor, G. R. Kline

Lattice dynamics of metals, semiconductors, quantum crystals (solid He^4); electron-phonon interaction and its relation to superconductivity (tungsten bronzes, $LaAl_2$, Zr_2Ni); structural phase transitions (tungsten bronzes, Zr); high temperature materials and properties including bonding and melting; effect of hydrogen and carbon impurities in metals (Th); structure and dynamics of electrolytic solutions (rare earth chlorides); magnetic structure of metals, in particular of rare earth metals and their alloys (Ho, Ce); electronic distribution in transition and rare earth metals and alloys (Cr-Mn, Lu, Yb).

6. MAGNETIC PROPERTIES OF SOLIDS $58,700 02-02
S. Legvold

Magnetic and transport properties of localized and conduction band (itinerant) electrons in rare earth metals and alloys; polarization of conduction electron bands via indirect exchange interactions (Gd-Y, Gd-Yb, Gd-Sc, etc.); valence fluctuations, crystallographic transformations (Ce, Ce-La, SmS); generalized susceptibilities as related to Fermi surface "nesting," magnetoresistance (Tb, Tb-Y, Tb-Th, Tb-Yb, etc.); magnetic scattering of conduction electrons in dilute 4f electron alloys (Y + Ce, La-Y + Ce, Lu + Ce); Cooper pair breaking in superconducting La containing magnetic impurities (La-Eu, La-Nd, La-Tb, etc.).

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

7. NUCLEAR RESONANCE IN SOLIDS $165,700 02-02
R. G. Barnes, F. Borsa,
Y. S. Hwang, D. R. Torgeson,
R. G. Lecander

Nuclear hyperfine interactions in solids, nuclear magnetic resonance, nuclear quadrupole resonance, nuclear Mossbauer effect; deuteron and transition metal NMR to characterize lattice sites and to study structural phase transformations and self-diffusion in transition metal hydride (VH_x, NbH_y, TaH_z) and deuteride phases (VD_x, NbD_y, TaD_z), to characterize lattice perfection and structural transformations in superconducting intermetallic compounds ($NbSe_2$, $TaSe_2$, $RhZr_2$), to investigate possible effect of charge density waves in one dimensional conductors (TTF-TCNQ) and in layer-compounds ($NbSe_2$, $TaSe_2$), and to investigate possible effects of spin-density waves in CrB_2.

8. SUPERCONDUCTIVITY $230,300 02-02
D. K. Finnemore, E. L. Wolf
J. E. Ostenson, M. Zaitlin,
P. S. Martinoli, J. R. Toplicar

Electron tunneling studies of the proximity effect; preparation of oriented superconductor-normal metal composites by directional solidification; Josephson tunneling in multilayer SNS junctions; flux pinning at planar superconductor-normal metal boundaries; superconducting transition temperatures near soft-mode crystal structure phase boundaries; effects on specific heat and magnetization of attractive interactions between quantized vortices; electron tunneling, Auger analysis and photoemission for getter sputtered A-15 superconducting films.

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

9. THERMODYNAMIC AND TRANSPORT PROPERTIES OF SOLIDS — $282,900 — 02-02
G. C. Danielson, A. J. Bevolo
H. R. Shanks, D. E. Eckels,
C. A. Swenson, M. S. Anderson,
G. L. Salinger

Electrocatalytic activity and surface properties of tungsten bronzes (H_xWO_3, Na_xWO_3, and K_xWO_3); Auger and SIMS studies of interfaces (Ta-Si and Au-Si) and hydrogen in WO_3, MoO_3, $LaNi_5$, and FeTi; heat capacity and superconducting transition temperatures associated with soft phonon modes and phase transitions in tungsten bronzes; crystal growth and sputtering of tungsten bronzes; thermal conductivity of vanadium; capacitance dilatometer thermal expansion measurements of silicon, terbium and gadolinium; high pressure studies of the specific heat of solid hydrogen, deuterium, and helium; precision thermometry, temperature scales.

10. OPTICAL AND SPECTROSCOPIC PROPERTIES OF SOLIDS AND LIQUIDS — $184,400 — 02-02
D. W. Lynch, C. G. Olson,
T. E. Furtak, F. H. Spedding,
A. Habenschuss, J. H. Weaver

Optical properties (transmission, reflection, thermoreflection, electroreflection) of solids in the near infrared, visible, and vacuum ultraviolet (using synchrotron radiation): Co, transition metal alloys and compounds (e.g., FeTi, Mo-Nb), A-15 compounds, noble metals, III-V, IV, and II-VI semiconductors; photoemission into liquid electrolytes; 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; Raman scattering and x-ray diffraction in aqueous solutions; HDO, D_2O, rare earth chlorides and perchlorates.

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

11. RARE EARTH METALS PREPARATION $128,000 02-02
K. A. Gschneidner, Jr.,
B. J. Beaudry, P. E. Palmer

Preparation of kilogram quantities of highly pure rare-earth metals (Sc, Y, La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu); preparation of single crystals of rare-earth fluorides (ScF_3, YF_3, LaF_3, CeF_3, PrF_3, NdF_3, GdF_3, TbF_3, DyF_3, HoF_3, ErF_3, LuF_3), metals (Sc, Y, Ce, Pr, Nd, Gd, Tb, Dy, Ho, Lu), and special alloys and compounds (Sc-Sm, -Eu, -Tm, and -Yb; Y-Sm, -Eu, -Tm, and -Yb; La-Ce, -Sm, -Eu, -Tm, and -Yb; Ce-Y, -Mg, and -Cu; Lu-Sm, -Eu, -Tm, and -Yb; Nd_2S_3, Gd_2S_3, and Er_2S_3); studies of new methods for preparation of highly-pure rare-earth metals in kilogram quantities.

12. OPTICAL AND SURFACE PHYSICS THEORY $93,000 02-03
R. Fuchs, K. L. Kliewer,
P. R. Rimbey, D. L. Johnson

Optical properties of metals, semiconductors, and insulators; studies of surfaces, thin films, small particles, and powders; effects of surface roughness, nonlocality, and local field corrections on optical properties and photoemission; collective excitations; phonons, plasmons, and excitons; photoemission into liquid electrolytes and catalysis; solar energy studies: photovoltaic cells and high-temperature absorbers.

13. SUPERCONDUCTIVITY THEORY $66,300 02-03
J. R. Clem, R. A. Klemm

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; critical currents and flux pinning in inhomogeneous superconductors; instabilities; ac losses.

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

14. MAGNETIC AND ELECTRONIC PROPERTIES OF SOLIDS THEORY — $100,700 — 02-03
S. H. Liu, B. N. Harmon, D. L. Johnson

Theory of soft modes, phonon anomalies, charge density waves, and displacive lattice transformations and their relation to the electronphonon interaction and superconductivity. High temperature materials and properties including bonding, melting, and ion transport. Induced and intrinsic magnetization densities in metals, compounds, and alloys; spin waves and other excitations in disordered systems; the d-f exchange interaction in rare earth metallic materials.

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

15. X-RAY AND NEUTRON CRYSTALLOGRAPHY — $261,700 — 03-01
R. A. Jacobson, J. E. Benson, B. J. Helland, F. Takusagawa

Development and extension of X-ray and neutron diffraction techniques; structural methods in the solid state; potential superconductors, metal complexes exhibiting weak solid state interactions, insecticides, unusual alkali metal species, coal characterization.

16. LOW OXIDATION STATES IN INORGANIC SYSTEMS — $94,900 — 03-01
J. D. Corbett, P. A. Edwards, J. Cline

Synthesis, structure and equilibrium reactions of metallic elements under anaerobic, high temperature, and reducing conditions (e.g., for Sc, Ti, Zr, Hf, Mo, rare earths); structures exhibiting metal-metal bonding, anisotropic conduction; homopolyatomic ions (e.g., of Sn, Sb, Pb, Bi, Te); ionic intermetallic phases.

17. CHEMISTRY OF HEAVY TRANSITION METALS — $133,400 — 03-01
R. E. McCarley, V. Katovic, M. S. Matson

Chemistry of heavy transition elements, especially Nb, Ta, Mo, W; synthesis 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.

18. LIQUID METALS — $57,800 — 03-02
R. G. Bautista, G. Burnet, M. J. Murtha

Heat capacities and heat content of liquid rare earth metals and alloys by levitation calorimetry; liquid metal purification by chemisorption on particulate solids.

AMES LABORATORY
Chemistry Division -03- (Continued)

19. METALS FROM FLY ASH $67,900 03-02
G. Burnet, M. J. Murtha

Recovery of alumina and iron oxide from fly ash using calcination, selective chlorination and hydrometallurgical processing.

20. THERMAL EMITTANCE PROPERTIES OF MATERIALS $30,900 03-02
R. G. Bautista

Normal spectral emittance of surfaces as a function of wavelength with emphasis on materials which absorb heavily at frequencies in the solar spectrum but have low emissivities in the blackbody spectrum at operating temperatures which permit their use in solar energy devices; quantitative characterization of surface roughness effect on normal spectral emittance of surfaces.

21. MASS TRANSFER AND TRANSPORT IN FLUIDS AND PARTICULATE SYSTEMS $104,400 03-02
L. E. Burkhart

Particle and fluid motion from numerical solution of the Navier-Stokes equations and from high-speed photography; motion and stability of fluids near free surfaces; transport near interfaces, especially drops and bubbles; particle size distribution and morphology in preparation of fine powders; reaction kinetics in multicomponent mass transfer systems involving chemical reaction.

22. HIGH TEMPERATURE CHEMISTRY $117,600 03-03
H. F. Franzen, M. Umana

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

AMES LABORATORY
Chemistry Division -03- (Continued)

23.	SURFACE CHEMISTRY AND CATALYSIS R. S. Hansen, B. C. Gerstein, K. G. Baikerikar, E. J. Derderian, R. C. Wilson	$262,400	03-03

Heterogeneous catalysis by metals and semiconductors with emphasis on clean surfaces; field emission microscopy, flash desorption spectroscopy, LEED and Auger spectroscopy, and single crystal face catalysis; electrical double layer properties and their alteration by absorption; mechanical and flow properties of interfaces; motion and electronic structure of surface adsorbed species as studied 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
N. L. Peterson - Phone: (FTS) 388-2222 or 312 739-2222

24. ALLOY PROPERTIES $467,000 01-01
F. Y. Fradin, A. T. Aldred,
D. J. Lam, B. W. Veal, Jr.,
G. Cinader

Electronic structure and its relationship to physical properties and bonding with emphasis on actinide compounds; preparation of thin film actinide compounds and studies of actinide solubility in glasses; magnetic properties of Np and Am compounds; XPS studies of oxides of U, Np, Pu, Am, Cm, and Bk; NMR studies of USn_3, $NpAl_2$, and $NpAl_3$; crystal-field calculations of Pu^{3+} magnetic form factors.

25. SCATTERING STUDIES $632,000 01-01
M. H. Mueller, G. H. Lander,
J. Faber

Magnetic and structural properties of actinide binary compounds using neutron and x-ray scattering; internal rearrangement of atoms accompanying magnetic transitions as well as x-ray evidence for strain effects; critical scattering near the ordering temperature; inelastic neutron scattering studies of magnetic excitations; hydrogen position parameters in storage metal hydrides; high-temperature structure of perovskite materials for MHD application; defect structure in doped ceria; pulsed neutron source for inelastic experiments on UO_2 and high-resolution powder unit for perovskite studies.

26. PHYSICAL METALLURGY $323,000 01-01
M. B. Brodsky, A. J. Arko
R. J. Trainor, Jr.

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, de Haas-van Alphen effect in actinide metals and compounds; scattering of electrons by lattice defects.

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

27. PROPERTIES OF HIGH-TEMPERATURE MHD MATERIALS — $69,000 — 01-01
A. T. Aldred, B. W. Veal, Jr., D. J. Lam, M. H. Mueller, J. Faber, Jr., W. L. Procarione

Studies of lattice and electronic structure of ceramic materials; electrical conductivity up to 1600°C and magnetic susceptibility up to 1000°C of $LaCoO_3$ and $La_{1-x}Sr_xCrO_3$; XPS studies of transition metal oxides and ABO_3 compounds (A = La, B = transition metal); x-ray and neutron diffraction studies of defects in $LaCoO_3$ and Ta_2O_5 doped ceria.

28. CATALYSIS AND SURFACE STUDIES — $31,000 — 01-01
M. B. Brodsky, R. J. Trainor, Jr.

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.

29. MECHANICAL PROPERTIES-PLASTICITY — $496,000 — 01-02
U. F. Kocks, A. P. L. Turner, R. A. Mulford, R. O. Scattergood, J. L. Routbort, H. Mecking, R. Labusch, R. Schwarz

Theoretical and experimental research on fundamental aspects of the mechanical properties of metallic and ceramic solids; computer simulations of the flow stress, strengthening mechanisms, dislocation motion through individual obstacles and random arrays; cyclic hardening and dynamic recovery, especially at elevated temperatures; constitutive relations for plasticity, creep and fatigue of metals and ceramics; structure characterization of deformed crystals by x-ray diffraction, electron microscopy, and internal friction.

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

30. MECHANICAL PROPERTIES- EROSION AND WEAR — $32,000 — 01-02
A. P. L. Turner, R. O. Scattergood

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.

31. METAL PHYSICS — $823,000 — 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, R. E. Einziger,
N. S. Choudhury, 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; tracer diffusion in Nb and W; mechanisms of ionic transport in solid electrolytes; transport properties and cation diffusion in oxides; hydrogen isotope diffusion in Nb; elastic and anelastic effects of interstitial impurities in transition metals.

32. SUPERCONDUCTIVITY — $260,000 — 01-03
F. Y. Fradin, G. S. Knapp
S. D. Bader, G. Cinader

Electron-phonon interaction in high transition temperature superconductors; NMR and Mossbauer effect studies of PdH (PdD) and Chevrel phases XMo_6S_8 (SMo_6Se_8) where X = Sm, Pb, or a rare-earth element; NMR studies of A-15 compounds, Chevrel phases, and C-15 Compounds $V_2Hf_{1-x}Ta_x$.

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

33. CHARGED-PARTICLE IRRADIATION — $525,000 — 01-04
K. L. Merkle, R. S. Averback, R. Benedek, R. L. Lyles, Jr., P. P. Pronko, K. H. Ecker

Study of defects and structures in recrystallized amorphous layers of ion implanted materials; channeling, blocking and elastic scattering analysis of defects and impurities in metals; studies of displacement cascade structures; correlation between 14 MeV neutron damage and heavy ion damage, sputtering; short range repulsive interactions in solids; properties of helium and hydrogen in metals and their interaction with lattice defects; heavy-ion damage in thin metal films; damage function studies; influence of ion channeling on defect production. Major experimental facilities include 300 keV heavy ion accelerator, STEM microscopy with in-situ ion irradiation capability, 14 MeV neutron source at LLL and high voltage electron microscopy (being procured).

34. NEUTRON IRRADIATION — $521,000 — 01-04
T. H. Blewitt, B. S. Brown, M. A. Kirk, Jr., B. A. Loomis, R. C. Birtcher

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)

35. KINETIC STUDIES $705,000 01-04
H. Wiedersich, F. V. Nolfi, Jr.
P. R. Okamoto, D. I. Potter,
M. D. Rechtin, A. Taylor,
S. P. Choi, G. R. Davidson,
R. J. DiMelfi

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; coagulation of insoluble gases in metals; stress fields around voids and their interaction with defects and other voids; the effect of fine precipitate dispersions, solute additions, helium, and projectile mass on void formation during ion bombardment; effects of interstitial loop structure and stress-induced preferred loop orientation on irradiation creep; damage structure produced during high-temperature ion bombardment of oxides; radiation sources include 300 KeV heavy-ion accelerator, 4 MeV Dynamitron, and high voltage electron microscope (being procured).

36. DIFFUSION STUDIES $128,000 01-04
R. W. Siegel, N. Q. Lam,
S. J. Rothman

Effects of irradiation on tracer diffusion in Ag and W; theoretical studies of solute segregation during irradiation.

ARGONNE NATIONAL LABORATORY
Solid State Science Division -02-
D. L. Price - Phone: (FTS) 388-3149 or 312 739-3141

37. NEUTRON SCATTERING STUDIES $1,045,000 02-01
T. Brun, J. M. Carpenter
G. Felcher, R. Kleb,
D. L. Price, S. K. Sinha
T. Worlton

Research is conducted in neutron inelastic scattering and neutron diffraction in magnetic systems and at high pressures; a major effort is dovoted to development and prototype testing of an intense pulsed spallation neutron source; steady-state and time-of-flight techniques are employed at the CP-5 research reactor while the spallation prototype employs the ZGS proton injector-booster. 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 diffusion of hydrogen in solid and liquid metals; the structure and lattice dynamics of hydrides; the dynamics of liquids including He^3; collective effects in the kinetic behavior of dense fluids; the dynamics and structure of amorphous and crystalline materials; 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.

38. MATERIALS SCIENCES RESEARCH WITH THE PROTOTYPE PULSED NEUTRON SOURCE (PPNS) $0 02-01
J. M. Carpenter, R. Kleb

The design and operation of PPNS as a prototype of the proposed Intense Pulsed Neutron Source (IPNS) and as a test bed for IPNS instrumentation; exploitation of the unique PPNS advantages of a large epithermal flux and short pulse width for elastic scattering studies at large momentum transfers (up to 80 Å) and for inelastic scattering at large energy transfers; materials to be investigated include superconductors, hydrogen storage materials, candidate MHD electrode materials, solid electrolytes, one-dimensional conductors and amorphous materials; to be initiated in FY 1977.

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

39. MATERIALS PREPARATION AND CHARACTERIZATION — $143,000 — 02-02
S. Susman, D. Hinks

Preparation of research samples of metal, insulator and semiconductor single crystals with documented physical and chemical properties; materials of current interest include alkali halides and cyanides, rare-earth hexaborides, and rare-earth compounds with CsCl and Ca_3Au structures; investigation of refractory oxides such as Y_2O_3 and CeO_2 in connection with MHD electrode problems; 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.

40. DEFECTS AND IMPURITIES IN NONMETALLIC SYSTEMS — $308,000 — 02-02
P. Yuster, C. Delbecq,
S. Marshall, J. McMillan

Study of defects and impurities in nonmetallic crystals and the processes caused by exposure of insulators to ionizing radiation emphasising the production and motion of vacancies and interstitials; electronic processes in refractory materials (Y_2O_3); structure and reorientation dynamics of molecular ion centers (Cl_2^-, $BrCl^-$) and heavy-metal-molecular-ion complexes ($ClSnCl^-$) in alkali halides; the effect of magnetic fields on recombination luminescence, ESR studies of impurities (Cr^{3+} in MgO and YAG, Gd^{3+} in ThO, Tl and Pb centers in KCl and radiation induced centers in lithium niobate, KDP, and triglycinsulphate), localized moments in alloys, the coordination of Cu^{++} in aminoacids, and temperature- and magnetic-field dependence of spin relaxation times.

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

41. LOW TEMPERATURE STUDIES $278,000 02-02
H. A. Kierstead, P. Roach
R. Webb

Studies of properties of quantum liquids and solids at very low temperature; precision measurements of the thermodynamic properties of He^3, He^4, and He^3-He^4 mixtures near phase transitions, properties of of superfliud phases of He^3, sound propagation and ion mobility in new He^3 phases, adiabatic cooling by nuclear demagnetization, specific heat measurements on Kondo systems (La:Ce); rare-earth sesquioxides displaying antiferromagnetic ordering, and mixed-phase alloys and compounds (Pb-Na, V_3Si, $V_3Sn_{0.5}Ga_{0.5}$, UAl_2 and USn_3).

42. SUPERCONDUCTIVITY STUDIES $346,000 02-02
R. Huebener, K. Gray
C. Falco, J. Hafstrom

Research in nonequilibrium processes in superconductors and the relation between metallurgical and superconducting properties in type II materials. Quantum interference effects, magnetic structures and transport properties of superconductors studied using high-resolution magneto-optical techniques, 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, and the preparation of high T_c materials by high-rate sputtering; development of high-temperature SQUIDS.

43. PHASE TRANSITIONS AND CATALYSIS $198,000 02-02
L. Guttman, D. O'Reilly

Phase transitions in order-disorder systems, the structure of glassy materials, the dynamics of molecules in amorphous systems and the properties of atoms and molecules adsorbed on surfaces studied with NMR, ESR and ENDOR spectroscopy. Computer modeling of liquids, amorphous solids and random network models of glasses; spin-echo measurements of self diffusion in H_2, D_2, and H_2-D_2 mixtures; the melting of quantum solids; magnetic resonance studies of surface states; diffusion of adsorbed species on surfaces and catalysis.

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

44. MAGNETIC PROPERTIES $150,000 02-02
T. O. Brun, B. D. Dunlap,
G. P. Felcher, G. K. Shenoy

Magnetic properties of metals, alloys and compounds are studied with emphasis on local-moment vs. itinerant models of magnetism; topics include Mossbauer effect measurement of hyperfine interactions, spin-lattice relaxation times and crystal-field effects in lanthanide and actinide materials; studies of the degree of localization 5f electrons in actinide laves phase intermetallics; measurements of crystal-field splittings and electronic relaxation effects in lanthanide cryolites; studies of rare-earth hydride and hydrogen; hyperfine interactions and electron relaxation effects in hemoglobin compounds; properties of dilute magnetic alloys employing neutron scattering, magnetization and specific heat measurements; local moment formation and the Kondo effect in Ce alloys and compounds such as $CeAl_3$, (La, Ce)Al_3 $CeSn_3$, $CePb_{3-x}Sn_x$ and $CeIn_{3-x}Sn_x$; competition between the Kondo effect and superconductivity in tunnel diodes made of $La_{1-x}Ce_xTh_y$; prototype studies of magnetic atomic-beam scattering from surfaces.

45. ELECTRONIC PROPERTIES $152,000 02-02
G. Crabtree, L. Windmiller

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 and studies of the scattering of electrons by impurities, lattice defects and local moments; experimental determination of g-factors at the Fermi surface in Au and complementary APW g-factor calculations; studies of conduction states with f-like character in the actinide compounds URh_3 and UGe_3; measurements of the Fermi surface in Mo, W and Nb and associated band structure calculations; Fermi surface studies of A15 compounds; scattering lifetimes in AuGa, Au, Pd, and Pt and dilute substitutional alloys of these hosts and studies of conduction electron scattering by vacancies introduced in Au and Pt and by dislocation loops in Cu.

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

46. LIGHT SCATTERING AND ACOUSTICS — $0 — 02-02
C. M. Falco, P. R. Roach, S. K. Sinha, P. H. Yuster

A program employing light scattering and acoustics to probe solids and liquids; light scattering investigations include: Raman scattering studies of vibrational modes of defects in insulators, local modes of mobile ions in superionic conductors, transport phenomena in refractory oxides and optic (hydrogen) modes in Pd and Nb hydrides and deuterides, as well as Brillouin scattering investigations of shear wave propagation in liquid crystals; acoustic studies include propagation of shear waves in liquid crystals and acoustic microscopy; to be initiated in FY 1977.

47. SOLAR MATERIALS — $0 — 02-02
C. J. Delbecq, J. A. McMillian, S. K. Sinha, D. Y. Smith, P. H. Yuster

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, Mie scattering in dielectric-colloid systems, theory of bulk and surface optical properties and sum-rule constraints, phase transformations in heterojunction solar cells, and charge transfer processes in organic photovoltaic materials; to be initiated in FY 1977.

48. REFRACTORY MATERIALS WITH MHD APPLICATIONS — $0 — 02-02
C. J. Delbecq, T. L. Gilbert, D. G. Hinks, S. A. Marshall, W. Primak, S. Susman, P. H. Yuster

Research in refractory materials including structural determination of conductive ceramics such as $La_{1-x}Sr_xCrO_3$ and $LaCoO_3$-$SrCoO_3$ solid solutions, studies of chemical reactions and equilibria at refractory surfaces exposed to high-temperature gases, electronic processes in refractory materials including Y_2O_3 and Al_2O_3, theoretical studies of interatomic forces and local electronic structure in oxides and preparation and characterization of research samples of high-temperature oxides such as Y_2O_3; to be initiated in FY 1977.

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

49. SOLID STATE THEORY $410,000 02-03
T. Arai, T. Gilbert,
D. Koelling, F. Mueller,
A. Rahman, J. Robinson
D. Smith, P. Vashishta

Theory of electron correlation; itinerant and local-moment theories of magnetism; electron-hole plasmas in semiconductors; hydrogen in metals; defects in metals and insulators; temperature dependence of magnetic ordering in rare-earth metals and alloys; localized ments and the Kondo effect; molecular dynamics calculations; theory of neutron scattering measurements; theory of liquids and vortex motion in quantum liquids; electron-phonon interactions; structure and interactions of atoms in molecules and solids; optical and electronic properties of insulators; electronic structure and properties of metals and intermetallic compounds; superconductivity and superfluidity; magnetism of transition metal alloys, surface phenomena.

50. PARTICLE SOLID INTERACTIONS $350,000 02-04
J. Jackson, W. Primak,
P. Vashishta

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 large-cluster impurity effects; field ion microscopy; metals currently under study include lead, platinum, rhodium, nickel, indium, mercury, molybdenum and tungsten; theoretical studies of defect formation and migration in metals; radiation damage in insulators includes work on lithium niobate, sapphire, spinel, lucalox, barium titinate, quartz, vitreous silica, and glasses; optical and electrical effects, dimensional changes, stress formation and relief migration of implanted ions to surfaces and voids, surface radiation damage, blister information 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

51. NEUTRON SCATTERING AND X-RAY DIFFRACTION STUDIES — $550,000 — 03-01
S. W. Peterson, M. Atoji, J. M. Williams, H. E. Flotow, E. G. Sherry, A. H. Reis, P. L. John, R. L. Musselman, R. Attig, M. E. Druyan

Chemical synthesis and materials evaluation (especially by neutron diffraction structure and bonding studies) of one-dimensional inorganic conductors such as the cation deficient Krogmann complexes; preparation and neutron structure study of complex organometallic hydrides of potential use in catalytic hydrogenation processes; neutron diffraction studies of rare earth compounds, metal carbides and sodium tungsten bronzes in high magnetic fields; neutron quasi-elastic scattering studies of Nb, V, Pd and Th hydride systems; X-ray structure and phase studies of hydride phases formed by trapping H or D in metallic films and of ion-bombarded materials of CTR interest; structure studies of hydrogen storage materials; structure and super-lattice studies of one-dimensional platinum oxalate complexes; structure and mechanistic studies of organophosphate extractants of actinide waste products of power reactors.

52. PHYSICAL AND SURFACE CHEMISTRY OF ENERGY SYSTEMS — $338,000 — 03-03
D. M. Gruen, R. L. McBeth, R. B. Wright, A. R. Krauss I. Sheft

Chemical effects of energetic reactive particle interactions with surfaces; mass and energy analysis of sputtered products; determination of ion-fraction sputtering yields; identification of molecular sputtered species using matrix isolation spectroscopy; measurements of chemical trapping efficiencies and elucidation of chemical trapping mechanisms in Ti, Si, Ge, SiC, Al_2O_3 and TiO_2; scanning electron microscope, ATR, Auger, ESCA and APS measurements of ion-implanted surfaces; laser Raman scattering studies of surface amorphitization and chemical species formed by ion implantation; photon absorption cross section measurements of metal atom impurities doped into solid deuterium matrices; photon absorption cross sections of transition-metal ions in fused salt solutions; elementary interaction energetics or organic molecules with metal atoms in argon matrices; glancing-angle X-ray diffraction studies of compounds formed by ion implantation.

ARGONNE NATIONAL LABORATORY
Chemistry Division -03- (Continued)

53. LOW TEMPERATURE CALORIMETRY $138,000 03-03
D. W. Osborne, H. E. Flotow
F. Grandjean, W. G. Lyon

Heat capacity measurement and determination of entropies, enthalpies, and Gibbs energies from 0.1 to 350K for use in thermodynamic calculations at higher temperatures; emphasis is placed on inorganic compounds of importance in 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 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.

54. HIGH TEMPERATURE CHEMISTRY $374,000 03-03
R. J. Thorn, R. J. Ackermann,
J. R. McCreary, E. G. Rauh
G. H. Winslow, G. E. Murch,
R. J. Tiernan, L. C. Wagner,
S. P. Garg

High-temperature thermodynamic, transport and 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; equilibrium thermochemical measurements to determine the structure-sensitive partial molar thermodynamic quantities; photoelectron spectroscopic investigations of valence-band electronic structures of solids; high-temperature X-ray diffraction measurements of thermal expansions and phase equilibria; equations of state studies and calculations related to lattice and crystalline potentials; investigations of atomic diffusion through computer-simulations and diffusion limited sublimation; studies of molecule-ions present during thermal excursions in reactors; investigations of condensation processes occurring in energy systems; evaluation of thermochemical systematics and data of lanthanide and actinide compounds and phases; materials studied: oxides, carbides, sulfides, fluorides of uranium thorium, plutonium, lanthanides, zirconium, silicon and aluminum.

ARGONNE NATIONAL LABORATORY
Chemical Engineering Division -03-
L. Burris - Phone; (FTS) 388-2579 or 312 739-2594
F. Cafasso - Phone: (FTS) 388-2579 or 312 739-2594

55. LIQUID METALS CHEMISTRY $210,000 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 Li-H_2, Li-D_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 and the Li-LiO_2 phase diagrams; distribution of oxygen, nitrogen and carbon between liquid lithium and selected lithium halide eutectic salts; study of binary Li-Li_2C_2 systems; interactions of lithium with refractory metals and alloys, corrosion mechanism of refractory metals and alloys in liquid lithium.

56. MOLTEN SALT CHEMISTRY $160,000 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; liquidus diagrams of multicomponent molten salt systems involving acidic salts such as $AlCl_3$ and $ZnCl_2$; thermodynamic and spectroscopic properties of salt vapors; identification of high temperature associated vapor species formed between acidic salts as $AlCl_3$, and $ZnCl_2$ with other salts; raman spectra of YCl_3 with alkali halides, spectra of $InAlCl_4$, $In(InCl_4)$, InCl, $CoBr_2 \cdot n\ AlBr_3$, $PdCl_2 \cdot n\ InCl_3$, $CuCl_2 \cdot n\ AlCl_3$; 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)

57. CHEMISTRY OF MATERIALS $160,000 03-02
P. T. Cunningham, B. Holt,
W. Hubble, 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 in Chicago, and St. Louis; IR method for quantitative measurement of acidic sulfate; attenuated total reflectance spectroscopy; stable isotope-ratio method for study of mechanisms of So_2 oxidation in atmosphere; nitrates, hydrocarbons, metals in chemistry of aerosols; 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, differential thermal analysis, X-ray diffraction and SEM studies.

58. THERMODYNAMIC PROPERTIES OF INORGANIC SUBSTANCES $270,000 03-02
P. A. G. O'Hare, W. N. Hubbard,
G. K. Johnson

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 ($\Delta H^{\circ}_{f(298)}$), high temperature enthalpy increments ($H_T - H_{298}$); 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, benzonapthofuran, chrysene, and (2) lanthanum, praseodymium, and neodymium trifluorides; calorimetric studies on $CaUO_4$, $MgUO_4$, γ-UO_3, UN, U_2N_3, ThN, $UO_2C_2O_4$, $UO_2(CH_3COO)_2$; ternary compounds of transuranium elements, e.g. Na_2PuO_4.

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

59. PHYSICAL CHEMISTRY OF ELECTRO-CHEMICAL ENERGY STORAGE — $110,000 — 03-02
R. K. Steunenberg, C. Melendres, M. Blander, M. Saboungi

Electrochemical and phase studies of electrode materials in lithium-aluminum/LiCl-KCl/metal sulfide batteries; electrode reaction kinetics and mechanisms; charge transfer processes; solid-state diffusion in lithium-aluminum; electronic and ionic conductivity; electromotive force measurements; lithium-aluminum, calcium-silicon, lithium-aluminum-calcium, and lithium-aluminum-indium alloys; 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; thermo dynamic properties of ternary alloys.

60. HEAT TRANSFER MATERIALS AND METASTABLE FLUIDS — $130,000 — 03-02
M. Blander

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; homogeneous and heterogeneous bubble nucleation and explosive boiling studies; P-V-T properties of stable and metastable fluids and testing of equations of state; contact vapor explosion mechanisms; nucleation theory; molecular dynamics, calculations; techniques for limit of superheat measurements of hydrocarbons; heterogeneous nucleation of water.

BROOKHAVEN NATIONAL LABORATORY
Upton, Long Island, New York 11973

Materials Science Division -C1-
D. H. Gurinsky - Phone: (FTS) 664-3504 or 516 345-3504
M. Suenaga - Phone: (FTS) 644-3518 or 516 345-3518

61. SUPERCONDUCTIVITY AND RELATIONSHIP BETWEEN PROPERTIES AND STRUCTURES — $700,000 — 01-03
M. Suenaga, A. Sweedler, T. Luhman, D. Dew-Hughes, C. Pande, R. Viswanathan, R. Caton, C. Klamut, O. Kammerer, D. Gurinsky

Fundamental properties of high critical temperature superconductors: long range order parameter, phase stability, stoichiometry, martensitic phase transformation, heat capacity measurements, neutron irradiation, x-ray and neutron diffraction, and normal state resistivity; preparation of high critical field, high current and critical current superconductors: preparation of multifilamentary A-15 superconductors, kinetics and mechanism of A-15 superconductors in solid state diffusion processes, relationship of microscopic defect structures to superconducting properties, stress induced phase transformation in A-15 superconductors, ac losses in Nb_3Sn.

62. RADIATION DAMAGE — $160,000 — 01-04
L. Snead, A. Sweedler, S. Moehlecke

Effects of different types of irradiation on critical properties of type II superconductors; resistivity and long-range-order effects in A-15 compounds; determination of damage effectiveness of 30-GeV and 17-MeV protons, and 14-MeV neutrons using superconducting critical-properties changes; defect studies using positron annihilation; defect structures and microstructure changes in irradiated type II samples; enhanced diffusion applied to A-15 fabrication.

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

63. NEUTRON SCATTERING - MAGNETIC SYSTEMS $510,000 02-01
G. Shirane, J. D. Axe,
L. Passell, R. A. Cowley
M. Iizumi, J. W. Lynn,
S. M. Shapiro

Neutron scattering studies on the structure and dynamics of magnetic materials: spin dynamics of substitutionally disordered antiferromagnets $Rb_2Mn_{0.5}Ni_{0.5}F_4$ and $Mn_{0.7}Zn_{0.3}F_2$; excitations in amorphous metallic ferromagnets; spin waves in ferromagnet CoS_2; spin density wave in Cr; magnetic ordering in $CsCoBr_3$; covalency effects in K_2IrCl_6.

64. NEUTRON SCATTERING - PHASE TRANSITIONS $490,000 02-01
S. M. Shapiro, J. D. Axe,
R. A. Cowley, G. Shirane,
M. Iizumi, J. W. Lynn,
J. Eckert, K. Carneiro,
R. Pynn, W. D. Ellenson

Neutron scattering studies of structural phase transitions and their dynamics; metal insulator phase transitions in NbO_2, charge ordering in the low temperature phase of magnetite, two-dimensional charge density waves in $NbSe_2$, Peierls transitions in one-dimensional conductors KCP and TTF-TCNQ.

65. NEUTRON SCATTERING - ELEMENTARY EXCITATIONS IN SOLIDS $435,000 02-01
J. D. Axe, S. M. Shapiro,
G. Shirane, J. Eckert,
K. Carneiro

Neutron spectroscopy of low-lying thermally excited energy states in solids; phonon dispersion in high density solid Ne grown at 6 Kbar; electron-phonon interaction in superconducting Nb, lattice dynamics of CuBr and AgBr.

BROOKHAVEN NATIONAL LABORATORY
Physics Department -02- (Continued)

66. NEUTRON SCATTERING - PARTIALLY ORDERED SYSTEMS — $380,000 — 02-01
L. Passell, K. Carneiro, H. Taub, W. D. Ellenson, J. D. Axe, S. M. Shapiro

Neutron scattering studies of short-range order and excitations in partially ordered systems; elastic scattering from monolayer N_2 on graphite, dynamics of monolayer Ar-36; anomalous inelastic scattering from ZrONb alloy; investigation of solid electrolytes such as β-alumina and BaF_2.

67. SUPERCONDUCTIVITY — $325,000 — 02-02
M. Strongin, D. L. Miller, R. Viswanathan, M. Yu, C. Varmazis, H. Lutz

Superconductivity in A-15 films; studies of normal state resistance in Nb_3Ge and Nb films; superconductivity in crystalline ultra-thin films; co-deposition of elements to study metastable phases in alloy films; ion-implantation in films; specific heat of thin film superconductors; non-equilibrium phenomena in superconducting weak links; conductivity of Bi filaments in the size quantization regime.

68. SURFACE STUDIES — $105,000 — 02-02
J. Strozier, M. Strongin, M. Yu, D. L. Miller

Use of ac techniques to study oxidation of CO on polycrystalline Pt and transition metal oxides; studies of desorption from surfaces under ion bombardment; use of LEED, AES, and secondary ion spectroscopy to characterize surfaces; studies of H^+ and H^- formation on surfaces; structural studies and surface phases.

69. LOW TEMPERATURE PHYSICS — $155,000 — 02-02
V. J. Emery, E. B. Osgood, W. C. Thomlinson

Study of the condensed phases of liquid helium, particularly the measurement of various properties of superfluid He-3 and the degelopment of a nuclear cooling apparatus for this purpose; neutron scattering studies of liquid He-3, helium films and solid mixtures of He-3 and He-4.

BROOKHAVEN NATIONAL LABORATORY
Physics Department -02- (Continued)

70. SPECTROSCOPY OF SOLIDS — 80,000 — 02-02
B. C. Frazer, H. Engstrom

Spectroscopic studies of structural, dynamic, and electronic properties of solids. Pre-construction R&D on the proposed synchrotron radiation facility. Light scattering, x-ray and dielectric experiments on substitutional impurity effects in ferroelectric KH_2PO_4; defect-induced Raman spectra from $NaClO_3$ and Al_2O_3; development of a new polarization technique for study of lattice defects and dilute impurity systems.

71. THEORETICAL RESEARCH — 385,000 — 02-03
M. Blume, G. J. Dienes, V. J. Emery, R. E. Watson, D. O. Welch, S. Krinsky, P. Bak

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; staggered magnetic fields in antiferromagnets; computer studies of one-dimensional and random magnetic systems; superfluidity in liquid He-3; analysis of soft x-ray photoemission data from alloys; dynamics and kinetics of crowdion interactions; defect-defect interactions and phase transitions; properties of superionic conductors; studies of valence electron distributions in crystals; Mossbauer and spin resonance line shapes and perturbed angular correlations in randomly varying external fields; fluctuations and surface superconductivity.

72. RADIATION EFFECTS RESEARCH — $440,000 — 02-04
A. N. Goland, P. W. Levy, K. J. Swyler, K. G. Lynn, R. Grynszpan

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; effects of radiation on thermal decomposition kinetics of ammonium perchlorate and other pseudostable solids; radiation-damage analysis for fusion and fission reactor materials studies.

BROOKHAVEN NATIONAL LABORATORY
Physics Department -02- (Continued)

73. PROPERTIES OF REAL SOLIDS — $420,000 — 02-04
A. N. Goland, P. W. Levy,
K. G. Lynn, H. Engstrom
C. Bottani

Utilization of particle-solid interactions as diagnostic probes in solid-state physics investigations; investigation of the properties of real solids; studies 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; ion implantation and Rutherford back-scattering experiments in superconductors; geological applications of mineral thermoluminescence.

74. ADVANCED MATERIALS SYNTHESIS AND CHARACTERIZATION — $115,000 — 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 and CTR systems; electrical conductivity, x-ray and neutron diffraction studies of pure and doped crystals of the $LaCrO_3$ system, $BaCeO_3$, $SrCeO_3$, $BaZrO_3$, $SrZrO_3$, $BaCoWO_6$, and Ba_2MnWO_6; structural studies of defect fluorites based on the ZrO_2 and CeO_2 system; x-ray studies of vapor deposited Nb-Ge alloys and synthesis of Nb_3Sn single crystals.

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

75. GEOTHERMAL SCALING AND CORROSION RESEARCH — $60,000 — 03-03
D. D. Keiser, D. E. Michels

Studies of physico-chemical processes which result in the deposition of solid materials along the flow path of the exploited geothermal water; development of analytical models; reactions between water and rock; corrosion of container materials; experimental vessels and conditions will be set up to produce scale materials important to geothermal systems; initial studies at temperatures below 300°F and pressures below 200 psi; deposition of $CaCO_3$ and mixed $FeCO_3$ and Fe_3O_4.

ILLINOIS, UNIVERSITY OF
Urbana, Illinois 61801

Materials Research Laboratory -02-
R. J. Mauer - Phone: 217 333-1370

76. ELECTRONIC STRUCTURE AND MAGNETISM OF TRANSITION METAL ALLOYS — $54,000 — 01-01
Paul A. Beck

Magnetic properties of copper-manganese and iron-aluminum 3d transition metal alloys with emphasis on magnetic structure of the "spin glass" or mictomagnetic alloys.

77. DYNAMIC STRUCTURE OF SUPERCRITICAL DENSE WATER AND AQUEOUS ELECTROLYTE SOLUTIONS — $42,000 — 01-01
J. Jonas

Nuclear magnetic resonance investigation of structure of aqueous solutions at high temperature and pressure with application to isotope separation.

78. PHYSICS OF REFRACTORY MATERIALS — $108,000 — 01-01
W. S. Williams

Investigation of the mechanical, electrical and catalytic properties of the transition metal carbides of columns IV, V, and VI of the periodic table; plastic deformation, surface hardness, and heterogeneous catalysis are related to electronic structure and lattice defects.

79. LOCALIZED CORROSION OF PASSIVE METALS — $14,000 — 01-01
R. C. Alkire

This project is a chemical engineering approach to localized corrosion and erosion of metal surfaces; associated investigations include stress corrosion cracking of titanium.

80. INTERSTITIAL SOLID SOLUTIONS — $52,000 — 01-02
C. J. Altstetter

The effect of oxygen on the mechanical properties of vanadium, niobium and tantalum; surface sputtering under energetic ion bombardment for compatibility as fusion reactor structural materials.

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

81. HYDROGEN BEHAVIOR IN BCC METALS — $127,000 — 01-02
H. K. Birnbaum

Behavior of interstitial hydrogen and helium in the bcc metals niobium, tantalum and vanadium; hydride precipitation and hydrogen embrittlement.

82. APPLICATIONS OF ELECTRON MICROSCOPY IN MATERIALS SCIENCE — $51,000 — 01-02
H. L. Fraser

Electron microscope investigation of the omega phase transition in zirconium-niobium alloys; precipitation of hydrides in niobium, hydrogen induced fracture of niobium, iodine embrittlement of zirconium.

83. DEFORMATION OF REINFORCED METALS — $34,000 — 01-02
M. Metzger

The development of realistic models of the mechanical behavior of metal composites using the Ni_3Al-Ni_3Nb aligned eutectic as a model system.

84. THE MECHANISM OF STRESS-CORROSION CRACKING - PROPAGATION STUDIES — $67,00 — 01-02
E. N. Pugh

The mechanism of stress corrosion cracking, both transgranular and intergranular, of alloys of magnesium, titanium and zirconium is investigated with emphasis on the role of hydrogen and the dynamics of crack propagation.

85. PRECIPITATION IN REFRACTORY METAL ALLOYS — $31,000 — 01-02
C. A. Wert

Carbide precipitation in binary alloys of vanadium and carbon, ternary alloys of vanadium-titanium-carbon and quaternary alloys of vanadium-titanium-chromium-carbon; emphasis is on the structure of precipitates, their stability, and their effect on mechanical properties.

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

86. DIELECTRIC SOLIDS — $57,000 — 01-03
D. A. Payne

Piezoelectric and pyroelectric dielectrics, both polycrystalline and single crystal are investigated to extend their useful properties to higher temperature applications; emphasis is on preparation by sintering and hydrothermal growth of bismuth and lead tungstate, titanate and germanate materials.

87. NUCLEAR MAGNETIC RESONANCE STUDIES OF METALS AND POLYMERS — $78,000 — 01-03
T. J. Rowland

NMR techniques are used to investigate the structure and mobility of the interstitial solutes, oxygen and nitrogen, in vanadium and other refractory metals, and hydrogen in niobium; the same techniques are used to determine molecular motion in crosslinked polymers.

88. PHYSICAL AND CATALYTIC PROPERTIES OF CATALYSTS — $11,000 — 01-03
G. P. Wirtz

Oxides are the focus of the research with emphasis on the properties of the rare earth perovskites which make them suitable for fuel cell electrodes and catalysts for hydrocarbon reactions and automobile exhaust oxidation; the thallium oxides are investigated for potential heat mirrors for solar energy applications.

89. USE OF VERY HIGH PRESSURE TO INVESTIGATE THE STRUCTURE OF MATTER — $121,000 — 02-02
H. G. Drickamer

High pressure in conjunction with resistivity, optical absorption and fluorescence measurements are used to probe the electronic structure and photochemistry of inorganic and organic materials; emphasis is on energy transfer reactions.

90. ANHARMONIC EFFECT IN SOLIDS — $108,000 — 02-02
A. V. Granato

Ultrasonic techniques are used to investigate the structure of interstitials in metals including hydrogen, the nonlinear elastic properties which determine the thermal behavior of materials, and dislocation properties which affect the strength of solids.

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

91. DEFECT PROPERTIES OF SOLIDS $95,000 02-02
D. Lazarus

Current research is on diffusion in body centered cubic transition metals like titanium and the mechanism of atomic mobility in superionic conductors like $RbAg_4I_5$ to determine if new defect models are needed for understanding these anomalous materials.

92. PROPERTIES OF NOBLE GAS CRYSTALS $93,000 02-02
R. O. Simmons

Quantum crystals like bcc ^3He are investigated to determine the quantum mechanisms of atomic mobility, the defect structure, the thermal properties, to characterize the phase transitions, and to explain the large lattice anharmonicities.

93. NUCLEAR MAGNETIC RESONANCE IN SOLIDS $168,000 02-02
C. P. Slichter

Current research centers on the related problems of the magnetic structure of transition metal atoms in alloys with nonmagnetic atoms and the explanation of the Kondo effect; on the structure and charge density waves in transition metal dichalcogenide layer compounds; and the electronic structure of platinum catalysts.

94. RADIATION DAMAGE IN SOLIDS $140,000 02-04
J. S. Koehler

The mechanism of defect production by high energy electrons and of defect annealing in body centered cubic and hexagonal metals are being studied with attention to the geometrical structure of the defects.

95. IMPURITIES IN SUPERCONDUCTORS $24,000 02-02
D. M. Ginsberg

Current research is focussed on the effect of hydrogen on the properties of superconductors using electron tunneling techniques.

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

96. RESPONSE OF SOLIDS TO ELECTRO-MAGNETIC RADIATION — $12,000 — 02-02
J. Dow

This project is a theoretical investigation of energy transfer processes involving radiation in solids, the optical characteristics of ultra transparent solids and the effect of large electric fields on optical properties; thermo-diffusion of electrical charge in metals and thermoelectric behavior are also studied.

97. LOW TEMPERATURE STUDIES OF DEFECTS IN SOLIDS — $30,000 — 02-02
A. C. Anderson

Low temperature techniques are used to investigate heat transfer in amorphous materials, heat transfer across interfaces both solid-solid and solid-liquid, mobility of interstitial hydrogen in bcc metals, dislocations and plasticity of superconductors, and atomic mobility in superionic conductors; significant attention is given to the development of low temperature technology.

LAWRENCE BERKELEY LABORATORY
University of California
Berkeley, California 94720

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

98. MICROSTRUCTURE PROPERTIES AND ALLOY DESIGN - ELECTRON DIFFRACTION AND MICROSCOPY — $270,000 — 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; structural investigations are carried out mainly by electron microscopy; systems under investigation include structural alloy steels, alloys undergoing spinodal and ordering transformations, and ceramics.

99. POWDER METALLURGY — $180,000 — 01-01
M. Pickus

Improve powder metallurgy processes to provide superior mechanical properties by reduced residual porosity; use the unique capability of the powder metallurgy process to provide materials essential to new energy systems and advanced technologies that cannot be produced by conventional methods.

100. THEORETICAL PROBLEMS IN ALLOY DESIGN — $185,000 — 01-02
J. W. Morris, Jr.

This program addresses key theoretical problems in the science of alloy design and draws on the results of this and other research for the synthesis of new materials to meet advanced engineering needs; problem areas include thermodynamics of alloys, correlation of microstructure to processing, correlation of mechanical properties to microstructure, and methods of synthesizing this information in the selection of alloy composition and processing.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

101. FUNDAMENTALS OF ALLOY DESIGN — $810,000 — 01-02
V. F. Zackay, E. R. Parker

Application of the principles of materials science and engineering to the design of complex multiphase alloys having increased cost effectiveness; control of microstructure through chemical composition and processing treatments to produce new materials with combinations of strength at room and elevated temperatures, corrosion resistance, fabricability, toughness, and other properties required by energy conversion systems components now under development. Determination of the mechanisms of erosion-corrosion in elevated temperature alloys subjected to the high temperature, erosive, reactive gas environments of coal gasification systems and direct coal fired turbine power plants; establishment of the role of alloying elements in resisting deterioration in gasifier environments and design of low cost alloys to resist degradation while retaining sufficient high temperature strength for service at temperatures of 1200°C.

102. RELATIONS BETWEEN DISLOCATIONS, POINT DEFECTS AND PROPERTIES OF CRYSTALLINE MATERIALS — $200,000 — 01-02
J. Washburn

Fundamental investigation of dislocation climb due to preferential capture of irradiation produced interstitial atoms in the 650 kV electron microscope; structure and nucleation mechanism of jogs and small dislocation loops in low stacking fault energy alloys; ion implantation damage in silicon and its recovery during low temperature annealing as revealed by electron microscope observation of the resulting secondary defects; development of mixed crystal $Zn_yCd_{1-y}S$-Cu_xS heterojunction solar cells with improved properties compared to the conventional CdS-Cu_xS solar cells; saturation of the radiation induced swelling in 316 stainless steel produced by 140 KeV protons at 625°C; electron microscope investigation of the mechanism of the shape memory effect in NiTi.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

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

The alloy systems niobium-tin, niobium-aluminum and niobium-aluminum-germanium are currently being studied; in each of these systems an A-15 compound occurs which has high values of the important superconducting parameters, critical temperature and critical field; the research involves two interdependent areas of study: the kinetics of forming the compounds, and the development of appropriate procedures for fabricating them into practical superconductors with maximum values of their respective superconducting properties; since these compounds are extremely brittle and powder metallurgy is particularly suited for coping with the problems encountered in the processing of brittle materials, the use of powder techniques is emphasized.

104.	MICROSTRUCTURE AND MECHANICAL BEHAVIOR OF CERAMIC MATERIALS: AND GLASS-AND CERAMIC-METAL SYSTEMS J. A. Pask	$145,000	01-03

Determination of phase equilibria, nucleation and growth phenomena in the SiO_2-Al_2O_3 system without and with small oxide additions; relationship of the character (particularly grain boundaries) of ceramic materials to their mechanical behavior at elevated temperatures; nature and reactions at glass-metal and ceramic-metal interfaces.

105.	HIGH TEMPERATURE REACTIONS A. W. Searcy	$187,000	01-03

Theoretical and experimental studies are being conducted in two related areas: the kinetics and thermodynamics of vaporization and of endothermic decomposition reactions, and the kinetics of transport of gases and vapors through porous solids.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

106.	RELATION OF MICROSTRUCTURE TO PROPERTIES IN CERAMICS R. M. Fulrath	$158,000	01-03

Densification of powder compacts which is of prime importance in the processing of ceramics and in powder metallurgy; these studies include systems where mass transport occurs in the solid state and when a liquid phase assists the process; development of thick film conductor systems with controlled microstructures to reduce or eliminate the precious metal content used in such systems; processing dictates the electrical properties.

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

Kinetics of crystallographic and microstructural changes in glassy carbon and correlation with conductivity, Hall coefficient, and magnetoresistance produced by heat treatment in the range 1000-3000°C; electrical properties of directionally solidified Al-$CuAl_2$ eutectic; microstructure, hardness and tensile properties of directionally solidified Al-Si eutectic.

108.	FAR INFRARED SPECTROSCOPY P. L. Richards	$140,000	02-02

Use of techniques of infrared spectroscopy, especially those of Fourier transform spectroscopy; specific projects include balloon flights to measure the sub-millimeter cosmic background radiation and to survey the sky for far infrared sources, studies of electron-hole droplets in optically pumped Ge, the use of photothermal ionization spectroscopy as an analysis tool for high purity Ge, magnetic surface modes in insulating antiferromagnets, spectroscopy of electronic states on the surface of liquid He, the development of ultra sensitive semiconducting and superconducting bolometer detectors.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

109. EXPERIMENTAL SOLID STATE PHYSICS AND QUANTUM ELECTRONICS — $175,000 — 02-02
Y. R. Shen

Use of modern optical techniques to study linear and nonlinear optical properties of materials, including gases, liquids, liquid crystals, and solids; new nonlinear optical phenomena in various materials with possible applications are being investigated.

110. EXCITED QUANTUM FLUIDS IN SOLIDS — 0 — 02-02
C. D. Jeffries

Study of phenomena that occur when light interacts with matter, in particular, semiconductors like Ge at low temperatures; electron-hole (e-h) Fermi liquid, a novel state of matter of high experimental and theoretical interest; phase separation, motion and surface tension of droplets, acceleration by strain gradients; alfven wave resonance, optical non-linearity, plasma resonance, magneto oscillatory phenomena, optical hysteresis and unusual explosive formation kinetics at high excitation powers; to be transferred to the materials sciences subprogram starting in FY 1977.

111. SUPERCONDUCTIVITY, SUPERCONDUCTING DEVICES, AND 1/f NOISE — $170,000 — 02-02
J. Clarke

Theoretical and experimental investigation of the phenomena of 1/f noise; origin of noise in metallic systems and semiconductors; development of a superconducting SQUID magnetometer that has a sensitivity of 10^{-10} GH$^{-1/2}$ at frequencies down to 10^{-2} Hz, and a drift of less than 10^{-10} G per hour; theoretical noise limitations of the dc SQUID; the dc SQUID is being incorporated in a new design of gradiometer to measure magnetic field gradients in surveying for geothermal sources and mineral deposits; this project is being undertaken in collaboration with Professor H. F. Morrison, and is supported in part by the USGS; in collaboration with Professor P. L. Richards we have constructed bolometers for far infrared measurements; development of bolometers for laboratory and astronomical measurements; non-equilibrium processes in superconductors; dissipation in superconductors.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

112. THEORETICAL SOLID STATE PHYSICS $40,000 02-03
M. L. Cohen

Theoretical studies of the electronic properties of solids; surface calculation on metals, semiconductors, solid-solid interfaces, steps and adsorbates; electronic calculations of chain, layer and narrow gap semiconductors; diamond and zincblende semiconductors, the superconducting polymer $(SN)_x$; the Si_2 molecule; Si vacancy; amorphous semiconductors.

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

Determination of the electrical, magnetic, and energetic changes in a solid that are associated with the change in volume; the volume changes are obtained by the use of high pressures.

114. LOW-TEMPERATURE PROPERTIES OF MATERIALS $125,000 03-01
N. E. Phillips

Low-temperature heat capacity measurements are used to obtain data that can be compared with microscopic or phenomenological theories of the properties of materials; the systems studied include superconductors, normal metals, magnetic materials, superfluids, and dielectric solids.

115. MASS AND CHARGE TRANSPORT IN ELECTROCHEMICAL SYSTEMS PROPERTIES OF NONAQUEOUS IONIZING SOLVENTS $115,000 03-01
C. W. Tobias

The combined effects of electrolyte and surface properties and of electrode geometry are studied under well defined hydrodynamic conditions in electrosynthesis, galvanic cells and in the shaping and finishing of metals; nonaqueous ionizing media are evaluated for use in extractive metallurgy and in galvanic cells; novel electrochemical process schemes of potential interest for the production of essential materials are explored.

116. HIGH TEMPERATURE THERMODYNAMICS $75,000 03-03
L. Brewer

Theoretical and experimental and spectroscopic and thermodynamic studies directed toward characterization of the high temperature behavior of condensed phases, particularly metals.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division (Continued)

117. CHEMISTRY AND MATERIALS PROBLEMS IN ENERGY PRODUCTION TECHNOLOGIES — $110,000 — 03-03
D. R. Olander

Gas-solid chemical kinetics by molecular beam mass spectrometry; laser vaporization of solids; radiation-enhanced gas phase and gas-solid corrosion reactions; high temperature behavior of nuclear fuels and fusion reactor materials.

118. CRYSTALLIZATION KINETICS — $85,000 — 03-03
L. F. Donaghey

Characterization of chemical processes for the preparation of solid-state materials for energy conversion application; of particular interest are processes for preparing crystalline films and coatings, such as chemical vapor deposition, reactive sputtering and liquid phase epitaxy.

119. ELECTROCHEMICAL PHASE BOUNDARIES — $125,000 — 03-03
R. H. Muller

Thin films and boundary layers at electrochemical interfaces are investigated for the purpose of increasing the efficiency of electrochemical processes for the storage, conversion and chemical use of electrical energy.

120. SOLID STATE AND SURFACE REACTION STUDIES — $225,000 — 03-03
G. A. Somorjai

Structure, chemical composition and oxidation state of surfaces and adsorbed gases; surface reactions and catalysis on crystal surfaces at low and at high pressures; solar energy conversion by photocatalyzed reactions of water and carbon dioxide; catalytic conversion of coal to liquid hydrocarbons.

121. NUCLEAR MAGNETIC RESONANCE — $90,000 — 03-03
A. Pines

New techniques in nuclear magnetic resonance; double-resonance and multiple-quantum transitions; study of microscopic structure and dynamics in ordered and partially ordered materials, for example, organic and inorganic solids and liquid crystals; conformation and structure of coal and oil shale; effect of nuclear spin on chemical reactions.

LAWRENCE LIVERMORE LABORATORY
P. O. BOX 808
Livermore, California 94550

G. Dorough - Phone: (FTS) 457-3767 or 415 447-3767
L. Roberts - Phone: (FTS) 457-7124 or 415 447-7124

122. HOT CORROSION STUDIES RELATED TO FOSSIL FUELS — $60,000 — 01-01
D. W. Short

Mechanisms and kinetics of hot corrosion (accelerated or catastrophic oxidation resulting from the added presence of a molten salt in an oxidizing atmosphere); Ni-base alloys in a Na_2So_4-O_2 environment; detailed analyses of the salt surface, salt-oxide interface, and oxide-alloy interface, and the substrate to determine the sequence of chemical reactions and the structural and morphological changes; transport through the salt; influence of gas composition; salt composition; electrochemical cell measurements; surface structure techniques such as X-ray photoelectron spectroscopy and Auger electron spectroscopy.

123. LOW INDEX MATERIALS (A) — $100,000 — 02-02
M. Weber, C. Cline

OPTICAL COATINGS (B) — $100,000 — 02-02
J. Khan, H. Levie

(A) Study of nonlinear optical properties and damage in materials subjected to intense light beams; refractive index nonlinearity measured using time resolved interferometry; glasses (simple and multicomponent), crystals (alkali halides, fluorides, oxides), and polymers (acrylic, polystrene); frequency dispersion response time; nonlinear porperties correlated with transmissive properties, UV and IR absorption; glass development based on Be fluoride.

(B) Amorphous and polycrystalline thin film structures; quantitative understanding of the factors that influence the properties of thin films; high energy electron diffraction; in-situ study of growing thin films; characterization of TiO_x as a function of process variables; in-situ stress measurements; optical coatings for laser applications.

LAWRENCE LIVERMORE LABORATORY (Continued)

124. D_2-DT-T_2 PHASE DIAGRAM $50,000 03-02
C. Souers

To determine the phase diagram of the 3 component system: D_2-DT-T_2; the region of greatest interest is the triple sufrace area of 18-21K; all data will be integrated into a theoretical framework that allows easy calculation throughout the phase diagram; to be measured; triple points by callibrated temperature sensors, vapor pressure by baratrons, gas phase equilibrium constants and kinetics by quadrupole mass spectrometer, liquid/solid equilibrium constants and kinetics by the nine-line fundamental infrared vibration rotation spectrum at 3-4.5um.

LOS ALAMOS SCIENTIFIC LABORATORY
University of California
P. O. Box 1663
Los Alamos, New Mexico 87544

CMB Division
R. D. Baker - Phone (FTS) 843-4563 or 505 667-4563
R. G. Bowman - Phone (FTS) 843-6014 or 505 667-6014

125. HIGH TEMPERATURE MATERIALS FOR ENERGY APPLICATIONS — $200,000 — 01-02
E. K. Storms, S. R. Skaggs
B. A. Mueller

Thermal stability of possible coating materials; measure and match coefficients of thermal expansion of protective coatings to possible refractory metal substrates; boron activity in various transition metal boride systems determined by high temperature mass spectrometry; data used to obtain phase relationships, thermodynamic properties and bond energies; data being used to interpret thermionic emission measurements and develop a bonding theory based on the Fermi energy.

126. HIGH TEMPERATURE NEUTRON DAMAGE STUDIES — $190,000 — 01-04
W. V. Green, D. M. Parkin
W. F. Sommer, M. L. Simmons
C. A. Coulter, L. S. Levinson

The LAMPF accelerator, its proton beam as a neutron simulation source and its beam stop as a neutron source; uniform heavy ion production in thick samples and concurrent gas and impurity atom production by 800 MeV protons; neutron and heavy ion primary recoils computed from nuclear data using NMTC, cross sections and thresholds; influence of neutron spectra on damage; voids and black spots produced by 800 MeV protons in thick high-purity Al; radiation hardening; internal friction; transmission microscopy of 800 MeV proton irradiated Al; preparation for a 10^{19} n/cm^2 irradiation; microhardness changes produced by 800 MeV proton; measurement of helium produced by LAMPF protons in Cu.

LOS ALAMOS SCIENTIFIC LABORATORY
CMB Division - (Continued)

127. CTR RELATED CHEMICAL RESEARCH TRITIUM CHEMISTRY ASSOCIATED WITH THE LITHIUM BLANKET AND CONTAINER MATERIALS — $140,000 — 03-02
J. L. Anderson, R. M. Alire, D. H. W. Carstens

Simultaneous measurement of diffusion coefficient and solubility of H_2 and D_2 in Li and its containers Nb and Nb-1%Zr; development of a diffusion model based on the combined radial and axial diffusion of H_2 into a solid cylinder to determine the solubilities and diffusion coefficients and testing of model by least-squares fitting of experimental data to the model; preliminary studies cover temperature range 1073 - 1373 K and pressure range 0.13 to 1330 Pa; extraction of tritium from molten Li using low melting eutectics containing Y, La and Ce; early emphasis on 84 at.% La-16 at .% Ni (mp $\sim$ 783K) eutectic; temperature coefficient for the liquid-liquid extraction and pressure-composition-temperature diagram for the appropriate metal-hydrogen systems under investigation; other eutectics under investigation include 84 at.% Ce-16 at.% Co. 82 at.% Ce-18 at.% Ni, 88 at.%Ce-12 at.% Fe, and 69 at.% Y-31 at.% Co.

Theoretical Division

127.5. LOS ALAMOS EQUATION OF STATE LIBRARY — $60,000 — 02-03
J. F. Barnes, G. I. Kerley

To develop an efficient and reliable search and interpolation program that can readily be used outside LASL for the LASL equation of state data; document the system and distribute the information to potential users; increase the number of materials represented by the tabular data, in accordance with the predominate user requirements.

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

128. LIQUID METALS RESEARCH $125,000 01-03
L. J. Wittenberg

Characterization of liquid metals and salts; liquid viscosity, electrical conductivity and thermal conductivity of liquid Ce and Pu; X-ray diffraction study of liquid Ce; application of hard sphere model of liquid metals to fused salts; electrotransport studies of lithium-hydrogen system.

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

Metals and Ceramics Division -01-
J. R. Weir, Jr. - Phone: (FTS) 850-1925 or 615-483-1925
C. J. McHargue - Phone: (FTS) 850-1278 or 615-483-1278

129. CERAMICS RESEARCH $329,000 01-01
C. S. Yust, J. Brynestad
S. L. Bennett, R. L. Beatty
H. P. Krautwasser

Structure of pyrocarbons; thermodynamics, structure and stability of tellurides; boron carbides, uranium nitrides and europium compounds; grain boundary structure and composition of ceramics; erosion of ceramics; mechanical properties of oxide-metal composites; microstructure of coal.

130. PREPARATION AND SYNTHESIS OF HIGH TEMPERATURE AND SPECIAL SERVICE MATERIALS $197,000 01-01
G. W. Clark, J. D. Holder
C. B. Finch, O. F. 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 and MHD devices; hydrothermally grown quartz; single crystals doped with lanthanides and actinides; study of edge-defined film-fed growth process; growth of large silicon crystals.

131. THEORY OF THE SOLID STATE $295,000 01-01
J. S. Faulkner, G. S. Painter
W. H. Butler, M. H. Yoo
B. Gyorffy, D. Hall
R. O. Jones

Aniesotropic elastic treatment of elastic energy of dislocations and 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; superconducint 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.

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

132. X-RAY DIFFRACTION RESEARCH $264,000 01-01
H. L. Yakel, Jr., B. S. Borie,
C. J. Sparks, Jr., R. W. Hendricks,
J. Hastings, J. Lin

Structures of Eu_2O_3; diffuse x-ray and neutron scattering measurements; study of forbidden Bragg reflections in hard superconductors; omaga-phase formation, transformations in uranium alloys; small angle scattering studies of voids in irradiated materials; inelastic resonance scattering; application of synchrotron x-radiation to study diffraction in solids.

133. DEFORMATION AND MECHANICAL PROPERTIES $300,000 01-02
R. A. Vandermeer, J. C. Ogle,
R. W. Carpenter, M. L. Grossbeck,
W. B. Snyder

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; recrystallization of rolled tantalum single crystals; role of grain boundaries on deformation processes; hydrogen embrittlement; microstructural aspects of erosion.

134. KINETICS AND MECHANISMS OF SURFACE AND SOLID STATE REACTIONS $460,000 01-03
J. V. Cathcart, R. E. Pawel
G. F. Petersen, R. A. McKee
T. S. Lundy, P. T. Carlson,
R. A. Perkins, C. L. White

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, 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; thermal gradient and stoichiometric effects on diffusion in UN; chemical and tracer diffusion in Fe-Cr-Ni; hydrogen isotopes in Cr_2O_3; interstitial solute atom-defect interactions in Nb and TiO_2; segregation of solutes to grain boundaries.

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

135. ENERGY TRANSPORT IN SOLIDS — $250,000 — 01-03
D. L. McElroy, R. K. Williams, J. P. Moore, T. G. Godfrey, T. K. Holder, J. Masey

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.

136. METALLURGY OF SUPERCONDUCTING MATERIALS — $310,000 — 01-03
C. C. Koch, D. M. Kroeger, D. S. Easton, D. J. Griffiths, A. Das Gupta

Effect of metallurgical variables on supersonducting 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 ($PbMo_6S_8$); $LiTi_2O_4$.

137. RADIATION EFFECTS — $1,260,000 — 01-04
J. O. Stiegler, K. Farrell, E. E. Bloom, D. S. Billington, J. M. Leitnaker, W. A. Coghlan, N. H. Packan, D. N. Braski L. K. Mansur, R. W. Carpenter, E. A. Kenik, M. B. Lewis, T. C. Reiley, M. Saltmarsh, G. Bauer, P. Jung

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.

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

138. ELEMENTARY EXCITATIONS IN CONDENSED MATTER — $570,000 — 02-01
W. P. Crummett, W. C. Koehler, H. A. Mook, R. M. Nicklow, H. G. Smith, N. Wakabayashi

Inelastic neutron scattering studies of phonons, magnons, excitons, and single particle excitations in solids, liquids, and gases; lattice dynamics of MnF_2, phonon spectra in molecular crystals, e.g., $NaClO_3$; phonon and magnetic excitations in EuO; interconfigurational fluctuations in $Sm_{1-x}Y_xS$; spin wave excitations in amorphous Ge; interband transitions in Si; high energy excitations in Ni; crystal field excitations in NdSb; inelastic scattering from noble gases; exchange interactions and anisotropy energies in rare earth-iron Laves phase compounds.

139. MAGNETIC PROPERTIES OF SOLIDS — $535,000 — 02-01
J. W. Cable, H. R. Child, L. David, W. C. Koehler, R. A. Medina, H. A. Mook, R. M. Moon, R. M. Nicklow

Elastic and inelastic scattering of polarized and unpolarized neutrons by magnetic systems; magnetic moment distributions in dilute and concentrated alloy systems Pd-Mn, Co-Cr, Co-Mn, Co-Ni, Co-V, Ni-Mn and Ni-Rh; form factors and spin densities in paramagnetic metals Sc, Tc, Y, and Nb; spin densities in cubic Laves phase compounds; configuration fluctuations in Ce-Th alloys, Ce-Al alloys and metallic Ce; magnetic critical scattering in Er, Gd, and Laves phase compounds; spin wave dispersion in Ni-V, Pd-Fe and Pt-Fe alloys; magnetic form factor of Fe, Ni and Gd from magnetovibrational scattering.

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

140. PROPERTIES OF DEFECTS, SUPERCONDUCTORS, AND HYDRIDES — $305,000 — 02-01
H. R. Child, D. K. Christen, W. C. Koehler, H. A. Mook, R. M. Nicklow, H. G. Smith, F. Tasset, N. Wakabayashi

Elastic, inelastic, and small angle scattering of neutrons by superconductors, organic conductors, superionic conductors, metal hydrides, and metals and compounds containing interstitial defects high resolution neutron inelastic scattering measurements of perturbations of phonon dispersion curves by radiation induced defects in Cu and Al; phonon spectra of high T_c superconductors; phonon anomalies in the Mo-Re and Cr-Re systems; phonon spectra of α-U; lattice dynamics of superconducting PdDx, dynamical properties of tritium in metal hydrides; temperature dependence of phonons in silver halides; lattice dynamical properties of TTF-TCNQ; phonon perturbations in simple salts by complex molecular impurities (CN^- in KCl); high frequency phonons in the Ta-D system; small angle neutron scattering by fluxoids in Nb and Nb-Ti alloys.

141. PHYSICAL PROPERTIES OF CERAMICS — $555,000 — 02-02
E. Sonder, J. B. Bates, Y. Chen, M. M. Abraham, J. C. Pigg, F. A. Modine, R. A. Weeks, G. E. Shankle H. D. Stidham, R. E. Frech

Effects of high temperature, particle and ionizing radiation on the optical and electrical properties and ion transport in crystalline and non-crystalline refractory materials such as MgO, Al_2O_3, $MgAl_2O_4$, and SiO_2; optical and electrical properties of solid state electrolytes and superionic conductors; 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)

142. PHYSICAL PROPERTIES OF SUPERCONDUCTORS — $350,000 — 02-02
S. T. Sekula, H. R. Kerchner, D. K. Christen, F. Tasset, H. G. Smith

Investigations of fluxoid morphology, fluxoid dynamics, and fluxoid-defect interactions in Nb-, V-, and Mo-base type-II superconducting alloys and A-15 compounds by dc magnetization, ac magnetic permeability, and flux-creep studies; small-angle neutron scattering by fluxoids in superconducting alloys and compounds; radiation and ion-implantation effects in type-II superconductors; neutron inelastic scattering studies of high-transition-temperature superconductors.

143. RESEARCH AND DEVELOPMENT ON PURE MATERIALS — $555,000 — 02-02
J. W. Cleland, G. C. Battle, W. E. Brundage, T. F. Connolly, C. C. Robinson, U. Roy, R. D. Westbrook, W. Uelhoff, F. James

Initial purification, single 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 and doped MgO, CaO, BaO, and SrO; electron beam float zone growth of refractory metals V, Nb, Zr, Ir and Re and their alloys; preparation of high purity Fe-Cr-Ni alloys, Ni-base alloys, Fe-base alloys, V-base alloys, and Mo-base alloys; preparation and characterization of Si crystals; single crystal growth of A-15 superconducting compounds and hexagonal Z-ferrites; preparation and synthesis of spinel titanates.

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

144. SURFACE STUDIES AND CATALYSIS — $310,000 — 02-02
L. H. Jenkins, D. M. Zehner, J. R. Noonan, J. F. Wendelken

Low energy ion damage to metal surfaces; sputtering of metals by high energy neutrons; studies of reordered metal surfaces and atomic site location using 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 and angular emission dependence in Auger spectra; true secondary electron emission and energy loss spectra variation with crystallographic effects; x-ray photoelectron spectroscopy (XPS), AES and LEED studies of chemisorbed overlayers on metal substrates; analysis of line shapes of secondary electron emission spectra from clean and adsorbate covered surfaces; examination of effects of surface electronic properties with respect to solid state aspects of heterogeneous catalysis.

145. PHOTOPHYSICAL PROCESSES OF SOLAR ENERGY CONVERSION — $320,000 — 02-02
R. F. Wood, J. W. Cleland, R. D. Westbrook, R. T. Young, J. B. Bates, B. R. Appleton

Characterization to determine the effects of point defects, defect clusters, dislocations, twins, stacking faults, grain boundaries, and unwanted chemical impurities in Si on electrical and optical properties; thermal neutron transmutation and chemical doping experiments to increase carrier concentration in Si without degrading carrier lifetime; electrical and optical (including laser-based infrared and Raman spectroscopy) property measurements on bulk specimens and test p-n junction diodes fabricated by evaporation, diffusion, and ion implantation; study of those factors known to degrade conversion efficiency, such as the voltage factor, charge loss due to surface recombination, and deviations from the ideal diode curve; theoretical band structure investigations; investigations of near surface properties of materials by ion implantation and ion backscattering; preparation, characterization and investigation of promising Group IV, III-V, and II-VI semiconducting materials; photophysical reactions in $NaClO_3$; photosensitive decomposition processes in perovskites and related compounds.

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

146. THEORY OF CONDENSED MATTER — $630,000 — 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, T. M. Wilson

Band structure calculations in metals and insulators; electronic properties of rare-earth and actinide compounds; electronic structure and optical properties of defects in insulators; mathematical modeling of photovoltaic devices; 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; hydrogen in 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.

147. LOW TEMPERATURE RADIATION EFFECTS — $430,000 — 02-04
R. R. Coltman, Jr., C. E. Klabunde,
J. K. Redman, J. M. Williams,
R. L. Chaplin

Interlaboratory program on 4°K damage rates in V, Nb, and Mo alloys; fission-neutron damage rates at 4°K in pure metals; irradiation methods for neutron scattering study of 4.9°K irradiated Cu; low-temperature recovery of thermal-neutron-irradiated high-purity V; resistance and magnetoresistance measurements of fast-neutron-irradiated pure and commercial Cu; correlated density and resistance measurements of fast-neutron-irradiated Cu; evaluation of a deuteron breakup neutron source for simulation of CTR radiation damage in Cu, Nb, and Pt; correlation of ion damage with fission-neutron damage in Al at 4°K.

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

148. X-RAY DIFFRACTION AND ELECTRON MICROSCOPY — $290,000 — 02-04
T. S. Noggle, S. M. Ohr
B. C. Larson, J. B. Roberto
J. Narayan, F. A. Sherrill

Radiation damage due to reactor neutron, 14 MeV neutron and ion irradiations of Au, Cu, Ni, Si and Nb; 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.

149. ION BOMBARDMENT — $245,000 — 02-04
B. R. Appleton, O. E. Schow III,
C. W. White, H. Verbeek
Q. C. Murphree, O. W. Holland
G. J. Clark

Optical emissions from ion-bombarded surfaces; characterization of stoichiometry and impurity depth profiles of high transition temperature superconducting Nb-Ge films by ion scattering, ion induced x-ray and resonant nuclear reaction techniques; hyperchanneling of 0.1-2.0 MeV H and He ions in Au, Ag and Si single crystals; experimental tests of electronic stopping theories in the velocity proportional region by channeling studies in Au single crystal films; radiative electron capture and bremsstrahlung of full stripped O ions channeled in Ag and Si single crystals; positive ion channeling spectroscopy of reordered and adsorbate covered surfaces.

150. NORMALIZATION OF ION AND NEUTRON DAMAGE — $125,000 — 02-04
T. S. Noggle, J. Narayan,
B. R. Appleton, J. A. Biggerstaff,
O. S. Oen, T. Iwata

Normalization of damage production rates using fission neutron and 5 MeV Al ion irradiation of thin films of Al; 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

151. CHEMICAL STRUCTURE OF ENERGY-RELATED MATERIALS — $630,000 — 03-01
W. R. Busing, G. M. Brown, C. K. Johnson, H. A. Levy, A. H. Narten, W. E. Thiessen

Atomic and molecular arrangements in crystals and in liquids determined by neutron diffraction and complementary x-ray diffraction studies; location of light atoms, especially hydrogen; development of new computational methods for solving refining, and interpreting crystal structures; use of intermolecular potentials to compute, predict, and extrapolate physical properties of liquids; materials studied include organic conductors and modulated structures, macromolecular catalysts for hydrogen production, molten salt catalysts for clean fuel synthesis, and salt hydrates for thermal energy storage.

152. BASIC MATERIALS CHEMISTRY RELATED TO FUSION REACTOR SYSTEMS — $400,000 — 03-02
J. T. Bell, F. J. Smith, J. D. Redman, G. M. Begun

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); acquisition of chemical data needed for design of effective tritium management schemes and to reduce inventory is the goal.

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

153. THERMODYNAMICS AND TRANSPORT IN MOLTEN SALTS AND HYDROUS MELTS — $127,000 — 03-03
J. Braunstein, A. L. Bacarella

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

154. SURFACE CHEMISTRY — $108,000 — 03-03
E. L. Fuller, P. A. Agron

Chemical and structural characterization of catalyst surfaces from 77°K to 1000°C; chemical reactivity and topology studied microgravimetrically, calorimetrically and spectroscopically; supported by theoretical, microscopic and mathematical analyses for more complete understanding of heterogeneous catalysis in commercial and pilot plant operations related to production of clean fuels from coal.

155. ELECTROCHEMICAL KINETICS AND CORROSION — $145,000 — 03-03
F. A. Posey, E. J. Kelly,
R. E. Meyer

Basic electrochemical mechanisms of corrosion reactions applicable to localized attack of metals (e.g., titanium) 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; magnetic field effects in electrode kinetics and corrosion; half-wave amalgamation potential of nobelium.

PACIFIC NORTHWEST LABORATORY
P. O. Box 999
Richland, Washington 99352
R. Nelson - Phone: (FTS) 444-2279 or 509 942-2279

156. CERAMICS FOR ENERGY APPLICATIONS — $100,000 — 01-01
T. D. Chikalla, R. P. Turcotte, L. C. Olsen

Radiation damage in fluorite crystal ceramics and glass; use of alpha emitters to study radiation damage and gas implantation; helium diffusion and inert gas trapping; metal-insulator-semiconductor photovoltaics; characterization of surfaces and interfaces; resistivity, Hall effect, Seebeck coefficient; single and polycrystalline silicon.

157. STRUCTURE-PROPERTY RELATIONSHIPS IN SPUTTER-DEPOSITED MATERIALS FOR SOLAR APPLICATIONS — $30,000 — 01-01
S. D. Dahlgren, R. P. Allen, R. Wang, W. T. Pawlewicz

Effect of grain structure on the electrical transport properties of silicon; cathodic sputtering; relationships of measured carrier mobility to grain structure; photolysis 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 $SrTiO_3$.

158. OPTICAL AND LASER MATERIAL STUDY — $50,000 — 02-02
J. S. Hartman, R. L. Gordon

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; 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.

PACIFIC NORTHWEST LABORATORY (Continued) -01-

159. OXIDATION, CORROSION, AND WEAR RESISTANT FINE-GRAINED MATERIALS — $30,000 — 01-03
R. P. Allen, M. D. Merz, R. D. Nelson

Study of sputter-deposited, oxidation, corrosion, and wear resistant materials; structure-property relationships; ultra-fine-grained and amorphous materials; extremely hard alloys and intermetallic components; pure metals; Fe-Cr-Ni and Ni-Cr with oxide dispersoids; WC, HfC, and BN.

160. SPUTTER-DEPOSITED SUPERCONDUCTOR RESEARCH — $100,000 — 01-03
S. D. Dahlgren, R. Wang

Study of sputter-deposited superconductors; cathodic sputtering; synthesis of new superconducting materials; relation of sputter-deposition parameter to properties; structure and stability of sputter deposits; role of additives such as oxygen; high-field A-15 compounds; Nb_3Al, $Nb_3(Al\text{-}Ge)$, Nb_3Ge, Nb_3Sn, Nb_3Gd, Nb_3Si.

161. TRANSURANIUM PHYSICAL METALLURGY RESEARCH — $230,000 — 01-03
R. D. Nelson, S. D. Dahlgren, M. D. Merz, R. P. Allen

Phase transformations in Pu; deformation processes in fine grained alpha Pu, coarse grained alpha Pu and sputter deposited Pu; creep of Pu allotropes; physical metallurgy of Np; self irradiation damage in Pu and Np metal; program concludes in FY-77.

162. RADIATION EFFECTS ON METALS — $350,000 — 01-04
J. L. Brimhall, H. E. Kissinger, P. L. Hendrick, E. P. Simonen, L. A. Charlot

Production, migration and annihilation or coalescence of irradiation produced defects; effect of helium on void nucleation in Mo and Ni; theoretical analysis of void coarsening behavior and void surface kinetics; analysis of Stage III annealing behavior in irradiated Mo; simulation of neutron radiation enhanced creep by light ions.

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

J. Galt - Phone (FTS) 475-4669 or 505-264-4669

163. DEFECTS AND IMPURITIES IN ION-IMPLANTED INSULATORS AND SEMICONDUCTORS — $60,000 — 01-03
P. Peercy, G. Arnold
G. Krefft, C. Norris

Depth-resolved and frequency-dependent cathodoluminescence; in-situ measurements of the lateral stress induced by volume changes in radiation-damaged near surface layers using the cantilever beam technique; optical properties and thermoluminescence of defects; thermal annealing and ionization-stimulated annealing; single crystal, polycrystalline and/or amorphous modification of SiO_2, Al_2O_3, TiO_2, Y_2O_3, MgO, Si_3N_4, CdTe, SiC, CdS and graphite.

164. SURFACE PHYSICS RESEARCH — $90,000 — 02-02
F. L. Vook, J. E. Houston,
J. A. Panitz, R. R. Rye,
P. J. Feibelman

Studies of organic adsorbates on refractory metal planes using field-desorption techniques; imaging gross structural details of biological molecules; true Auger lineshape for the $L_{2,3}$ VV transition from clean Si surface; construction of a low temperature (4.2°K) field-desorption spectrometer designed specifically for organic and biological imaging; electron spectroscopic data of molecular interactions with metal surfaces.

SANDIA LABORATORIES (LIVERMORE)
Livermore, California 94550

B. Murphey - Phone (FTS) 469-2884 or 415 455-7011

165. GASES IN METALS $50,000 01-02
H. J. Saxton, G. J. Thomas,
W. A. Swansiger, W. D. Wilson

Experimental and theoretical aspects of H and He interactions in solids; influence on mechanical properties; diffusion, trapping and clustering of He in metals and alloys; He introduced by T decay; theoretical calculations of activation energy for He migration and energies of binding of He to simple defects; transmission electron microscopy; tensile testing of bulk samples; diffusion and trapping of H; Ni.

SECTION B

Universities

The information was taken from current 200-Word Summaries provided by the contractor. There is considerable (about 10%) turnover in the University program and some of the projects will not be continued beyond the current contract period.

ARIZONA STATE UNIVERSITY

201. SOLID STATE CHEMISTRY OF RARE EARTH OXIDES — $55,000 — 03-01
L. Eyring - Dept. of Chemistry

Defect structure in rare earth oxides, x-ray and neutron scattering, high resolution electron microscopy of selected oxides; studies of non-stoichiometry and structural analysis of oxide phases during compositional changes.

202. IMAGING SURFACES AND DEFECTS IN CRYSTALS — $52,244 — 02-02
J. M. Cowley - Physics Dept.

Development and application of electron microscopy for investigating chemical reactions at surfaces-such as oxidation of metals and reduction of ceramic oxides; techniques used-diffraction, diffraction-reflection and scanning electron microscopy.

203. STUDY OF FERRITE FORMATION IN NEUTRON IRRADIATED AUSTENITIC STAINLESS STEELS — $28,938 — 01-04
J. T. Stanley - Engineering Mechanics, Materials & Measurements Dept.

Experimental study of neutron radiation-induced ferrite formation in heat treated austenitic stainless steels; techniques used-transmission electron microscopy; magnetization.

BROWN UNIVERSITY

204. A COMBINED MACROSCOPIC AND MICROSCOPIC APPROACH TO THE FRACTURE OF METALS — $85,000 — 01-02
J. Gurland and J. R. Rice - Division of Engineering

Experimental and analytical studies of deformation and fracture in metals, primarily steels, including crack initiation and growth, particle rupture and/or interface decohesion, and void formation during high temperature creep; techniques used-mechanical testing, quantitative metallography, finite element analysis, crystal plasticity modeling.

CALIFORNIA INSTITUTE OF TECHNOLOGY

205. STUDIES OF ALLOY STRUCTURES AND PROPERTIES — $170,000 — 01-01
P. Duwez - Division of Engineering

Characterization of structure and properties of amorphous alloys obtained by extremely rapid solidification; effect of B, P, C, or Si on electrical resistivity and magnetic susceptibility of Fe-Ni-Co-base alloys; superconductivity and superconductivity-to-normal transition in binary LaAu and Gd-Au alloys.

206. METALS HYDRIDES WITH MULTIPLE PULSE NUCLEAR MAGNETIC RESONANCE TECHNIQUES — $53,397 — 03-01
R. M. Vaughan - Chemistry and Chemical Engineering Department

Application of multiple pulse nuclear magnetic resonance techniques to study chemical bonding and electronic structure in selected binary hydrides; double resonance techniques applied to heavy metal ions.

UNIVERSITY OF CALIFORNIA/LOS ANGELES

207. HIGH TEMPERATURE IRRADIATION DAMAGE AND PRECIPITATION HARDENING IN NI-BASE ALLOYS — $75,000 — 01-02
A. J. Ardell - Materials Department

Experimental investigation of irradiation induced defects, specifically in Ni-base alloys at elevated temperatures; effects of additions of solutes (Al, Ti, Si, and Cr) on void formation and γ' precipitation; techniques used-transmission electron microscopy, N^+ and Ni^+ ion irradiation.

208. FOURIER SPACE COMPUTER SIMULATION OF CRYSTALLINE IMPERFECTIONS — $38,800 — 01-01
D. de Fontaine - Materials Department

Theoretical studies of defect stability in elastic continuum; order-disorder transformations and associated phase diagrams for binary systems, using cluster variation methodology; vacancy concentration profiles near grain boundaries in irradiated material.

UNIVERSITY OF CALIFORNIA/RIVERSIDE

209. THEORETICAL ASPECTS OF SUPERCONDUCTOR — $77,000 — 02-03
E. Simanek - Physics Department

Theoretical study of order parameter fluctuations in superconductors and charged superfluids; electron-phonon coupling; order parameter-charge density coupling.

UNIVERSITY OF CALIFORNIA/SAN DIEGO

210. THE RESPONSE OF SUPERCONDUCTORS TO VARIATIONS IN IMPURITY CONTENT AND APPLIED PRESSURE — $125,122 — 02-02
M. B. Maple - Physics Department

Measurements of superconductivity at high pressures and in various types of materials - Kondo systems with local impurity-induced magnetic perturbations and multiple transition temperatures superconductors containing rare-earth impurities, high transition temperature A15 compounds, soft superconductors (Zn, Cd, and Al), and lamellar graphitic compounds.

211. RESEARCH ON THE PROPERTIES OF MATERIALS AT VERY LOW TEMPERATURES — $214,000 — 02-02
J. C. Wheatly - Physics Department

Experimental investigation of liquid ^{3}He; superfluid properties; non-linear response to and propagation of magnetic disturbances; static and dynamic nuclear magnetism; techniques used-ultrasonic atten attenuation, magnetization.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA

212. RESONANCE STUDIES OF SUPERIONIC CONDUCTORS — $41,392 — 02-02
V. Jaccarino - Physics Department

Experimental study of superionic conductivity of perovskite and fluorite structures using magnetic ions and decay of electronic spin correlation functions as a probe of activated motion; local phenomena at electrode-electrolyte interfaces; techniques: nuclear magnetic resonance, electron paramagnetic resonance.

CARNEGIE-MELLON UNIVERSITY

213. GENERALIZATION OF INTERNAL CENTRIFUGAL ZONE GROWTH OF METAL-CERAMIC COMPOSITES — $36,346 — 01-01
R. F. Sekerka - Metallurgy & Materials Science Department

Analysis of the internal centrifugal zone growth (ICZG) crystal growing process for refractory materials and composites; theoretical modeling of the directional solidification crucibleless process; experimental research to confirm model predictions of the effects of dimensionless variables.

CASE WESTERN RESERVE UNIVERSITY

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

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. DISLOCATION-SOLUTE ATOM INTERACTIONS IN ALLOYS — $53,000 — 01-02
R. Gibala - Metallurgy and Materials Science Department

Evaluation of strengthening mechanisms in refractory metals containing interstitial solutes; solute-solute and solute-dislocation interactions; relationship of microscopic interactions to macroscopic flow properties; effect of surface films and solute gradients on strength, techniques used-mechanical testing, internal friction, electrical resistivity, transmission electron microscopy.

CASE WESTERN RESERVE UNIVERSITY (Continued)

216. EXPERIMENTS IN HIGH VOLTAGE ELECTRON MICROSCOPY — $77,000 — 01-04
T. E. Mitchell - Division of Metallurgy and Materials Sciences

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

217. 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

Experimental investigation of stress corrosion cracking of stainless steels in aqueous chloride environments; effect of elastic strain and prior plastic deformation on electrochemical parameters such as potentials for cracking, pitting, and corrosion.

UNIVERSITY OF CHICAGO

218. THE STUDY OF PHONONS AND ELECTRONIC PROCESSES IN ORDERED AND DISORDERED SOLIDS — $55,000 — 02-02
S. A. Solin - Physics Department

Optical studies of disordered solids, using laser Raman spectroscopy; low frequency Raman scattering in glasses; coordination dependent vibrational properties of amorphous alloys; forward scattering measurements on Ge(As); electrical and optical properties of graphite intercalates; Brillouin spectrum of NiF_2.

UNIVERSITY OF CINCINNATI

219. FLUX PINNING AND FLUX FLOW STUDIES IN SUPERCONDUCTORS USING FLUX FLOW NOISE TECHNIQUES — $39,000 — 02-02
W. C. H. Joiner - Physics Department

Measurement of voltage fluctuations generated by fluxoid motion in type II superconductors; effects of cold work surface and volume pinning, and surface coatings on fluxoid-induced noise; pinning force on flux bundles.

UNIVERSITY OF CINCINNATI (Continued)

220. RADIATION EFFECTS ON BCC REFRACTORY METALS AND ALLOYS — $44,000 — 01-04
J. Moteff - Materials Science and Metallurgical Engineering Department

Experimental study of microstructural stability and high temperature mechanical properties of irradiated refractory metal alloys (Mo, Nb, W); comparison of fast neutron (fluence $\geq 10^{22}$/ cm^2) with heavy ion radiation on dislocation loop and void formation and swelling kinetics; correlation of hot hardness with tensile and creep properties; techniques used-mechanical tests, transmission electron microscopy, electrical resistivity, heavy ion accelerators.

CLARKSON COLLEGE OF TECHNOLOGY

221. NUCLEATION OF VOIDS — $22,990 — 01-04
J. L. Katz - Chemical Engineering Department

Theory of nucleation of voids and other defect precipitates such as interstitial loops; radiation effects in metals; hydrogen attack; effects of stress, inert gases such as helium and gases which can undergo simultaneous chemical reaction such as dissolved atomic hydrogen combining to form molecular hydrogen or reacting with carbon to form methane.

UNIVERSITY OF COLORADO

222. CRITICAL SCATTERING OF LASER LIGHT BY BULK FLUIDS AND THIN FLUID FILMS — $59,200 — 02-02
R. Mockler and W. O'Sullivan - Physics and Astrophysics Department

Experimental and analytical study of intensity autocorrelation measurements of critical fluid mixtures and thin fluid films; anomolous index of refraction of critical fluids using precision Fabry-Perot interferometer.

COLORADO SCHOOL OF MINES

223. LIQUID LITHIUM CORROSION AND CORROSION-FATIGUE RESEARCH — $46,094 — 01-01
D. L. Olson & D. Matlock - Metallurgical Engineering Department

Investigation of corrosion of ferrous alloys by molten lithium; kinetics of weight loss and grain boundary penetration as affected by stress, contact potential, nitrogen contamination, and chromium concentration.

COLUMBIA UNIVERSITY

224. HIGH TEMPERATURE TRANSPORT PROPERTIES AND PROCESSES OF GASES AND ALKALI METALS — $47,066 — 03-02
C. F. Bonilla - Chemical Engineering Dept.

Measurements of liquid compressibility and of vapor pressure of cesium, soidum and lithium to the critical point; studies of surface tension of liquid lithium, and interfacial and wetting studies in liquid-metal molten salt systems; heat transfer characteristics of hydrogen, hydrogen-carbon monoxide mixtures, and superheated steam.

UNIVERSITY OF CONNECTICUT

225 ELECTRODE POLARIZATION STUDIES IN HOT CORROSION SYSTEMS — $41,200 — 01-01
O. F. Devereux - Metallurgy Department

Experimental study of the corrosion of metals (Fe, Cr, Ni) and steels (plain carbon and stainless grades) in molten salts; measurement of polarization curves in salts with various hydrogen, sulfur and oxygen activities; evaluation of surface morphology and surface and subsurface corrosion products.

226. ELECTRON-DISLOCATION INTERACTIONS AT LOW TEMPERATURES — $41,075 — 01-02
J. M. Galligan - Metallurgy Department

Electron drag on dislocations plastic behavior of pure metals and alloys in the vicinity of their superconducting transition temperatures; dislocation-flux line interactions in superconductors; dislocation-interstitial interactions; Pb, Pb-Sn, Pb-Ag alloys and Nb.

227. CLUSTER CARBURIZING — $39,097 — 01-01
J. E. Morral - Metallurgy and Institute of Materials Sciences Dept.

Experimental study of carburization of metal alloys; precipatate-carbon and solute-carbon interactions; cluster carburizing concept in Ta-Hf and Nb-Hf alloys.

CORNELL UNIVERSITY

228. INFLUENCE OF GRAIN BOUNDARIES ON THE ELECTRICAL TRANSPORT PROPERTIES OF POLYCRYSTALLINE SI FILM — $25,000 — 01-01
D. G. Ast - Materials Science and Engineering Department

Experimental study of grain boundaries in pure and doped silicon; fabrication of specimens with controlled boundary orientations using Schober-Balluffi technique or CVD; transmission electron microscopy characterization of boundary structure; electrical measurements planned on specimens with selected boundary configurations; project started in FY 76.

229. STRUCTURE AND PROPERTIES OF OF GRAIN BOUNDARIES — $82,000 — 01-01
R. W. Balluffi - Materials Sciences and Engineering Department

Experimental study of grain boundary structure and properties in Au alloys; segregation and distribution of solute atoms in alloyed systems; boundary diffusion; boundary faceting and preferred orientation; techniques used-x-ray diffraction, Auger electron spectroscopy, thin film methods, and electron microscopy.

230. REDUCTION OF MIXED SPINEL OXIDES — $42,375 — 01-01
L. C. DeJonghe - Materials Sciences and Engineering Department

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.

231. ENVIRONMENT AND FRACTURE — $59,000 — 01-02
H. H. Johnson - Materials Sciences and Engineering Department

Experimental and theoretical investigations of hydrogen effects in body-centered-cubic (iron and niobium-base) alloys; permeation of hydrogen and deuterium in niobium; trapping sites in steels after various thermomechanical treatments; transmission microscopy characterization of changes in dislocation substructure after hydrogenation; theoretical analysis of hydrogen supersaturation produced by dislocation and bulk transport.

CORNELL UNIVERSITY (Continued)

232. THEORY OF STRUCTURE AND DYNAMICS IN CONDENSED MATTER — $120,000 — 02-03
J. A. Krumhansl - Atomic and Solid State Physics Laboratory

Analyses of structural changes near phase transitions and of coupled electronic and structural transitions in anisotropic solids; computer simulation; theory of disordered systems; application of electronic and lattice theories to computation of macroscopic properties, such as elastic constants.

233. MECHANICAL BEHAVIOR OF MATERIALS AND STRUCTURAL ELEMENTS AT ELEVATED TEMPERATURES — $60,000 — 01-02
R. H. Lance - Theoretical and Applied Mechanics Department

Development of constitutive equations describing elevated temperature mechanical response of structural elements such as beams and cylinders; equation-of-state concepts; creep and stress relaxation under various loading sequences in aluminum and stainless steel.

234. MECHANICAL PROPERTIES OF CRYSTALLINE SOLIDS — $63,077 — 01-02
C. Li - Materials Science and Engineering Department

Experimental and analytical study of mechanical properties of crystalline solids at high temperature; plastic equation of state; tensile, creep, load relaxation, and anelastic deformation modes in lead and stainless steels; design of accelerated testing techniques.

235. PROBABILISTIC MODELS OF THE STRESS-RUPTURE OF COMPOSITE MATERIALS — $31,500 — 01-02
S. L. Phoenix - Sibley School of Mechanical & Aerospace Engineering

Mathematical analysis of time-dependent mechanical behavior of composites; stress rupture properties of fiber-reinforced polymers; model based on fiber fracture statistics and matrix viscoelasticity; project started in FY 76.

CORNELL UNIVERSITY (Continued)

236. EXPERIMENTAL PHONON PHYSICS $250,000 02-02
R. O. Pohl and A. J. Sievers--
Laboratory of Atomic and Solid
State Physics Department

Calorimetric and spectroscopic studies of amorphous and highly disordered crystalline solids; effects of neutron irradiation on amorphous materials; lattice dynamics and surface phonon modes in crystals; far infrared properties of glasses and semiconductors.

237. DEFECTS IN METAL CRYSTALS $180,000 01-04
D. N. Seidman - Materials Sciences
and Engineering Department

Characterization of structure of and defects in metals using field ion microscopy; range of collision - replacement sequences, depleted zone structure, and interaction between self and gas-impurity interstitials in irradiation induced defects in Mo, W, Pt, and stainless steel alloys; construction of Poschenrieder lens for of atom probe field ion microscopy.

DARTMOUTH COLLEGE

238. THEORY OF ELECTRON-PHONON SCATTERING EFFECTS IN METALS $28,097 02-03
W. E. Lawrence - Physics and Astronomy
Department

Analyses of electron-phonon scattering effects, transport coefficients, and superconducting properties in metals; anisotropic quasipasticle and transport relaxation times in noble and polyvalent metals; non-equilibrium electron distributions in thermal gradients; evaluation of diffusion model applicability modelling of effective mass enhancement and superconducting gap anisotropies.

DARTMOUTH COLLEGE

239. EXPERIMENTAL DETERMINATION OF THE TEMPERATURE DEPENDENCE OF METALLIC WORK FUNCTIONS AT LOW TEMPERATURES — $28,323 — 02-02
P. B. Pipes - Physics and Astronomy Dept.

Measurement of temperature dependence of contact potentials in both normal and superconducting metals-Nb primarily, but also Cu, Au, Ag, Al, Zn, Pb; effects of superconducting-normal transitions and adsorbed gas layers; (He and Ne); theoretical analysis of effect of adsorbed gas on work function.

DREXEL UNIVERSITY

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

Experimental study of strain hardening in iron; deformation by wire drawing, strip drawing, and combination of these; tube drawing; dislocation configurations and mobility.

UNIVERSITY OF FLORIDA

241. QUANTITATIVE ANALYSIS OF SOLUTE SEGREGATION IN ALLOYS BY TRANSMISSION ELECTRON MICROSCOPY — $42,500 — 01-01
J. J. Hren and C. S. Hartley - Metallurgical and Materials Engineering Department

Simulation and evaluation of defect images in transmission electron microscopy; effect of solute segregation on local strain fields around dislocations and precipitates, based on continium elasticity and representation of dislocation as a summation of infinitesional displacements; experimental evaluation of planar defects in Si and precipitation in Al alloys.

UNIVERSITY OF FLORIDA (Continued)

242. DEFORMATION PROCESSES IN REFRACTORY METALS — $40,000 — 01-02
R. E. Reed-Hill - Materials Sciences and Engineering Department

Experimental investigation of dislocation-impurity interactions in niobium and, to a lesser degree, titanium; dynamic and static strain aging in niobium containing hydrogen and oxygen impurities; dislocation substructure and fracture morphology evaluation using transmission and scanning electron microscopy.

GEORGIA INSTITUTE OF TECHNOLOGY

243. INVESTIGATIONS OF RELATIONSHIPS BETWEEN MICROSTRUCTURE, MAGNETIC PROPERTIES AND THE HYDRIDING PROCESSES IN INTERMETALLIC COMPOUNDS OF RARE EARTH AND TRANSITION METALS — $60,000 — 01-01
B. R. Livesay - Applied Sciences Laboratory

Magnetic property measurements as a function of H content in FeTi and $LaNi_5$; hydriding and dehydriding to be followed with microstructural measurements and magnetic properties; the effect of surface conditions and prior thermal-mechanical treatments on the hydriding-dehydriding process; in-situ study of hydride nucleation.

GEORGETOWN UNIVERSITY

244. THE STUDY OF VERY PURE METALS AT LOW TEMPERATURES — $70,000 — 02-02
W. D. Gregory - Physics Department

Superconductivity in pure metals; experimental and theoretical studies of properties of inhomogeneous and non-equilibrium type-I superconductors; electrical conductivity; microwave transmission; laser irradiation effects; thin films; aluminum, tin, and gallium-indium alloys.

UNIVERSITY OF HAWAII

245. PRESSURE DERIVATIVES OF ELASTIC MODULI IN B.C.C. TRANSITION METALS AND THEIR SOLID SOLUTIONS — $37,804 — 02-02
M. H. Manghnani - Geology and Geophysics Department

Determination of pressure dependence of the elastic constant, lattice parmeters of the pressure induced transformations in bcc refractory metals V, Nb, Ta, Mo, and W; techniques used-hydrostatic pressure, ultrasonic methods, x-ray diffraction, laser heating.

UNIVERSITY OF HAWAII (Continued)

246. PHOTOELECTRIC EMISSION FROM THIN FILMS IN THE VACUUM ULTRAVIOLET REGION — $32,500 — 02-02
W. Pong, Physics and Astronomy Department

Experimental study of photoemission alkali and alkali-earth halides, oxides, nitrides, and organic superconductors to determine band structures density of states, bandwidths and thresholds; optical spectra of solid surfaces and thin films; electronic structure of polar insulators.

UNIVERSITY OF HOUSTON

247. MICROSTRUCTURAL STUDIES OF HYDROGEN AND OTHER INTERSTITIAL DEFECTS IN BCC REFRACTORY METALS — $53,500 — 02-02
S. C. Moss and W. R. McIntire - Physics Department

Experimental study of single crystal vanadium containing hydrogen (or deuterium), oxygen, and/or nitrogen to evaluate lattice distortion and occupany sites associated with interstitials interstitial effect on metal electronic structure; techniques used-x-ray and neutron diffraction and γ-ray Compton profile measurements.

HOWARD UNIVERSITY

248. RADIATION DAMAGE IN OPTICALLY TRANSPARENT MATERIALS (ZIRCONS) — $20,000 — 02-04
A. N. Thorpe - Physics Department

Measurements of optical absorption spectrum, low temperature anisotropic magnetic susceptibility, electron spin resonance, and thermoluminescence of zircon crystals subjected to alpha particle, gamma ray, and/or neutron radiation.

ILLINOIS INSTITUTE OF TECHNOLOGY

249. THERMAL AND ELECTRICAL MEASUREMENTS ON SOLIDS AT LOW TEMPERATURES — $193,954 — 02-02
H. Weinstock - Physics Department

Measurement of thermal conductivity of dielectric materials (MgO, Al_2O_3, and Al_2MgO_4), superconducting Pb-base alloys, ultrapure V, Kondo alloys, amorphous Ge and Si, thin (1 to 10 micron) metal films, and polymers; effects of ion bombardment and fission and 14 MeV neutrons; specific heat of Si, Ge, and antiferromagnetic insulators.

UNIVERSITY OF KANSAS

250. HIGH TEMPERATURE CHEMISTRY $60,401 03-03
P. W. Gilles - Chemistry Department

Vaporization behavior of high temperature substances, including studies of congruency and of non-stoichiometry; synthesis and vaporization of rare earth borides, and analysis of the ternary system boron-sulfur-silicon; relationships between structures of condensed phase and gaseous species.

LEHIGH UNIVERSITY

251. PRESSURE SINTERING AND CREEP DEFORMATION - A JOINT MODELING APPROACH $47,550 01-01
M. Notis - Metallurgy and Materials Sciences Department

Correlation of the kinetics of later stages of desification by pressure sintering with creep deformation; determination of rate-controlling mechanisms; effects of stress, temperature, microstructure and stoichiometry; quantitative relationships via deformation maps; CoO and $MgAl_2O_4$.

MARQUETTE UNIVERSITY

252. DEFECT STRUCTURES IN NONSTOICHIOMETRIC OXIDES $69,047 01-01
R. N. Blumenthal - Mechanical Engineering Department

Defect structure, thermodynamics and electrical transport correlations in pure and doped nonstoichiometric oxides; electrical conductivity, transference numbers by electrochemical cells, and thermogravimetric analysis; effects of temperature, oxygen partial pressure, dopant valence, ionic radius, and concentration; CeO_2 doped with CaO, ThO_2 and Ta_2O_5.

UNIVERSITY OF MARYLAND

253. AN INVESTIGATION OF IRRADIATION STRENGTHENING OF BCC METALS AND SOLID SOLUTIONS — $52,000 — 01-02
R. J. Arsenault - Chemical Engineering Department

Experimental investigation of effects of neutron irradiation and dissolved inert gas on the mechanical properties of body-entered cubic refractory metals (V and Nb) containing various levels of oxygen; low temperature reactor irradiation; introduction of helium into niobium through tritium permeation and subsequent decay; kinetics of gas bubble formation; techniques used-mechanical tests, electrical resistivity, transmission electron microscopy.

254. ALLOY STRENGTHENING DUE TO ATOMIC ORDER — $30,900 — 01-02
M. J. Marcinkowski - Mechanical Engineering Department

Mathematical modeling of macroscopic and microscopic deformation and crack formation in metals, using differential geometry and continuum elasticity techniques; calculation of dislocation configurations and interaction between passing dislocations in both ordered and disordered structures.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

255. HIGH TEMPERATURE PROPERTIES AND PROCESSES IN CERAMICS — $92,000 — 01-03
H. K. Bowen, B. J. Wuensch
Ceramics Department

Thermomigration in ceramics; theory and experiment; oxygen tracer diffusion; kinetic and thermodynamic factors; nonstochiometric oxides; UO_2 and UO_2-CeO_2 solid solutions.

256. THERMAL NEUTRON SCATTERING STUDIES OF MOLECULAR DYNAMICS AND CRITICAL PHENOMENA IN FLUIDS AND SOLIDS — $80,000 — 02-01
S. H. Chen, S. Yip
Nuclear Engineering Department

Coherent quasi-elastic neutron scattering from simple solids such as Rb and Ar near their melting points to evaluate local structural relaxation; diffusion coefficients in gas mixtures of Xe in H_2 or He, using light scattering methods; effect of pressure and composition fluctuations.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (Continued)

257. THE LUMINESCENCE PROCESS IN CHEMICAL REACTIONS — $57,235 — 03-03
L. Gole - Chemistry Department

Study of the formation and structure of metal clusters and other high temperature species; laser-induced fluorescence and chemiluminescence methods for study of electronically excited states of matter; determination of latent heats of sublimation, vaporization; selected state activation energies from intensity measurements of beam-gas chemiluminescent reactions.

258. BASIC RESEARCH IN CRYSTALLINE AND NONCRYSTALLINE CERAMIC SYSTEMS — $408,000 — 01-01
W. D. Kingery, R. L. Coble - Metallurgy and Materials Science Department

Broad program on basic studies in ceramic systems; electrical conductivity of doped UO_2; irradiation enhanced sintering; microstructure effects on Al_2O_3 properties; chemical transport at grain boundaries; solute-lattice defect interactions in MgO; influence of strain energy on the exsolution of solutes in single crystal MgO; shell model calculations of point defect energies of formation and association in MgO; creep and strength of SiC and Si_3N_4.

259. LOW TEMPERATURE AND NEUTRON PHYSICS STUDIES — $93,598 — 02-01
C. G. Shull - Physics Department

Study of the diamagnetic neutron scattering by Bi and of the de Haas van Alphen effect in nearly perfect Cu crystals; development and application of neutron interferrometry, using phase interference.

MICHIGAN STATE UNIVERSITY

260. PROPERTIES OF RARE GAS SOLIDS — $99,607 — 02-02
G. L. Pollack - Physics Department

Experimental study of thermal conductivity in single crystalline argon and molecular solids such as Kr and N_2; rare gas interactions with membranes and organic solids; phonon dynamics and scattering from defects; effects of condensed surface He layers on the kapitza resistance of Cu.

MICHIGAN TECHNOLOGICAL UNIVERSITY

261. A STUDY OF GRAIN BOUNDARY SEGREGATION USING THE AUGER ELECTRON EMISSION TECHNIQUE — $56,252 — 01-02
D. F. Stein, L. A. Heldt - Metallurgical Engineering Department

Grain boundary segregation in metals and effect on properties; stress corrosion cracking, theory and experiment; Auger photoelectron spectroscopy; sulfur segregation in Mo bicrystals; Bi in Fe; S in Fe; stress corrosion cracking of brasses; hydrogen embrittlement of copper alloys and pure iron.

UNIVERSITY OF MINNESOTA

262. ANALYSIS OF THE DUCTILE-BRITTLE TRANSITION TEMPERATURE IN FE-BINARY ALLOYS — $42,100 — 01-02
W. W. Gerberich - Chemical Engineering and Materials Sciences Department

Evaluation of flow and fracture in binary iron-nickel and iron-silicon alloys including ductile-brittle transition, strain-rate sensitivity, dislocation dynamics, and fracture morphology; techniques used-mechanical tests, accoustic emission, stress relaxation.

263. EXPERIMENTAL INVESTIGATIONS IN SOLID STATE AND LOW TEMPERATURE PHYSICS — $176,877 — 02-02
A. M. Goldman, W. V. Weyhmann, and W. Zimmerman, Jr. - Physics Department

Study of fluctuations in superconducting-to-normal transition, including measurement of pair-field susceptibility and specific heat of superconducting films; magnetism in kondo systems, using SQUID magnetometer, liquid and solid helium research involving lambda transition; critical points of $^{3}He/^{4}He$ mixtures; quantum properties of the superfluid component of ^{4}He; low temperature specific heat of crystalline ^{3}He.

UNIVERSITY OF MINNESOTA (Continued)

264.	IN-SITU ELECTRON MICROSCOPE INVESTIGATION OF THE NUCLEATION AND GROWTH OF SPUTTERED THIN FILMS T. E. Hutchinson - Chemical Engineering and Materials Sciences Department	$41,030	01-01

Nucleation and growth kinetics of vacuum deposited thin films; ultra high vacuum in situ electron microscopy, effects of substrate, temperature, deposition rate, pressure, and residual gases; Au on Si, CdS on Si.

NATIONAL ACADEMY OF SCIENCES/NRC - NATIONAL MATERIALS ADVISORY BOARD

265.	CONTINGENCY PLANS FOR CHROMIUM UTILIZATION	$50,000	01-01

Multitask study to be done in cooperation with other Federal agencies to address the technical alternatives and economic feasibility of replacing chromium throughout the economy.

NATIONAL ACADEMY OF SCIENCES/NRC

266.	AN ASSESSMENT OF THE NATIONAL NEED FOR FACILITIES DEDICATED TO THE PRODUCTION OF SYNCHROTRON RADIATION C. K. Reed - Solid State Sciences Committee	$24,850	02-02

Study of the scientific opportunities available through the use of synchrotron radiation; assessment of current facilities and future needs.

STATE UNIVERSITY OF NEW YORK/STONY BROOK

267. APPLICATIONS OF MICRODYNAMICS AND LATTICE MECHANICS TO PROBLEMS IN PLASTIC FLOW AND FRACTURE — $54,000 — 01-02
J. C. Bilello - Materials Sciences Department

Experimental and theoretical investigation of deformation and cleavage in refractory metals (Mo and W); surface energy and plastic relaxation measurements; effects of interstitial and substitutional impurities; analyses of surface energy in ionically bonded solids and neutron scattering and phonon dispersion associated with dislocation core structure; techniques used-mechanical tests, position annihilation, internal friction, and etch pit analysis.

UNIVERSITY OF NORTH CAROLINA

268. INVESTIGATION OF DEFECT STRUCTURES BY ELECTRIC POLARIZATION AND RELAXATION METHODS — $79,000 — 02-02
J. H. Crawford, Jr. - Physics and Astronomy Department

Impurities and point defects and their interactions in ionic crystals; kinetics of formation, decomposition, reorientation and transport of impurity-defect complexes; ionic thermocurrents; optical absorption and radiation effects; SrF_2: Gd^{3+}, CaF_2: U^{3+}: H^- and CaF_2: H^- systems.

NORTH CAROLINA STATE UNIVERSITY

269. SORPTION OF CESIUM BY GRAPHITES AT HIGH TEMPERATURES — $48,194 — 03-03
L. Zumwalt - Nuclear Engineering Department

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.

NORTHWESTERN UNIVERSITY

270. EFFECT OF POINT DEFECTS ON MECHANICAL PROPERTIES OF METALS — $53,500 — 01-04
M. Meshii - Materials Sciences Department

Experimental investigation of mechanical behavior of body-centered-cubic metals (Fe and Nb); effect of interstitials produced by electron irradiation or impurities on dislocation motion, macroscopic yielding, and work hardening or softening; techniques-mechanical tests, 2Mev Van de Graaff accelerator, transmission electron microscopy.

271. BASIC RESEARCH ON CERAMIC MATERIALS FOR ENERGY — $65,000 — 01-01
D. H. Whitmore - Materials Sciences Department

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; alkali titanates, germanates, and stannates; mixed chlorides.

OHIO STATE UNIVERSITY

272. FUNDAMENTAL STUDIES OF METAL FLUORINATION REACTIONS — $54,200 — 01-03
R. A. Rapp - Metallurgical Engineering Department

Experimental investigation of the thermodynamics and kinetics associated with fluorination of metals, initially nickel; solubility in and diffusion of fluorine to be measured using potentiostatic electrochemical methods; electrical conductivity and defect structure of fluorides to be characterized; extension of above data to fabricate a fluorine activity cell.

273. HYDROGEN ATTACK OF STEEL — $39,821 — 01-02
P. G. Shewmon - Metallurgical Engineering Department

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

OHIO STATE UNIVERSITY (Continued)

274. CORROSION, STRESS CORROSION CRACKING, AND ELECTROCHEMISTRY OF THE IRON AND NICKEL BASE ALLOYS IN CAUSTIC ENVIRONMENTS — $52,500 — 01-01
R. W. Staehle and A. K. Agrawal - Metallurgical Engineering Department

Evaluation of corrosion cracking of metals (Fe, Mo, Ni, and Cr) and their alloys in caustic environments; corrosion kinetics; effect of inhibitors on corrosion kinetics and polarization curves; stress corrosion cracking in aqueous caustic environments.

OKLAHOMA STATE UNIVERSITY

275. ELECTRONIC STRUCTURE OF DEFECTS IN OXIDES — $23,400 — 02-02
G. P. Summers - Physics Department

Experimental investigation of defects in oxides (CaO, SrO, ZnO, and Al_2O_3) after irradiation with γ-rays, electrons, or protons; trapping characteristics and electronic structure of defects in pure and doped oxides; techniques used-photoconductivity and optical absorption.

PENNSYLVANIA STATE UNIVERSITY

276. CERAMIC RESEARCH — $32,642 — 01-02
R. C. Bradt, J. H. Hoke - Materials Sciences Department

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 MgO $\cdot x$ Al_2O_3 spinel.

277. STUDIES OF MECHANICAL PROPERTIES AND IRRADIATION DAMAGE NUCLEATION OF HTGR GRAPHITES — $29,800 — 01-04
P. A. Thrower - Material Sciences Department

Experimental project determining effect of boron on radiation damage in pyrolytic graphite up to 1400°C; stress-enhanced oxidation of extruded graphite up to 1200°C in gas mixtures containing various CO_2, CO and H_2O levels; residual strength of graphite after different preexposures.

PENNSYLVANIA STATE UNIVERSITY (Continued)

278. STRUCTURE OF GLASSES CONTAINING TRANSITION METAL IONS — $50,000 — 01-01
W. B. White - Materials Research Laboratory

Structure and stability of insulator glasses with transition metal oxide additions; degree of order, structure of modifier and transition metal site, kinetics of phase separation and crystallization; Raman spectroscopy, optical absorption, luminescence, x-ray diffraction and electron microscopy; silicate, borate, borosilicate, germanate and phosphate glasses with Cr, Fe, Mn, and Ni oxide additions.

PURDUE UNIVERSITY

279. TRANSPORT AND THERMODYNAMIC PROPERTIES OF SOLIDS — $40,000 — 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 analysis and scanning electron microscopy; Cu-Ni-Zn, Fe-Ni-Al, and Fe-Ni-Cr ternary systems.

280. HIGH TEMPERATURE EFFECTS OF INTERNAL GAS PRESSURES IN CERAMICS — $52,421 — 01-03
A. A. Solomon - Nuclear Engineering Department

Effects of pore-entrapped gases and microstructure on rate-controlling mechanisms of pressure induced densification and swelling of ceramics; single and polycrystalline CoO.

RENSSELAER POLYTECHNIC INSTITUTE

281. THE EFFECT OF WELDING VARIABLES ON THE SOLIDIFICATION SUBSTRUCTURE, MECHANICAL PROPERTIES AND CORROSION BEHAVIOR OF AUSTENITIC STAINLESS STEEL WELD METAL — $43,300 — 01-01
W. F. Savage, D. J. Duquette - Materials Division Department

Corrosion and stress corrosion cracking of steels in wrought and welded conditions; pitting; effects of weld-parameters, solution pH, chloride concentration, impurity and segregation at ferrite/austenite interphase boundaries, and high pressure.

RENSSELAER POLYTECHNIC INSTITUTE (Continued)

282. FATIGUE BEHAVIOR OF BCC METALS — $29,700 — 01-02
N. S. Stoloff - Materials Engineering Department

Fatigue behavior of b.c.c. metals; effects of microstructural, testing and environmental parameters; hydrogen effects; high cycle (stress-controlled) and low cycle (strain-controlled) conditions; dislocation substructure and second phase effects; room temperature and above; V, Nb, V-H and Nb-H alloys.

UNIVERSITY OF ROCHESTER

283. THE MATERIALS AND MECHANICS OF OF RATE EFFECTS IN BRITTLE FRACTURE — $42,703 — 01-02
S. J. Burns - Mechanical and Aerospace Sciences Department

Experimental and analytical study of crack growth in steel and brittle polymers; critical stress intensity; grain size effects; ductile-brittle transition; dynamic fracture criteria.

284. DIFFUSIONAL CREEP OF MULTI-COMPONENT SYSTEMS — $37,500 — 01-02
J. C. M. Li - Mechanical and Aerospace Sciences Department

Measurement of creep of metals and polymers, using penetration creep method; plastic zone size; modeling of hydrogen embrittlement, radiation damage, and interaction of interstitial impurities with internal stress fields.

UNIVERSITY OF SOUTHERN CALIFORNIA

285. ELECTRICAL AND MECHANICAL PROPERTIES OF OXIDE CERAMICS — $55,435 — 01-03
F. A. Kroger - Electronic Sciences Laboratory

Electrical conductivity, transference number, and creep as function of oxygen pressure, dopant concentration, temperature, and grain size, determination of rate controlling point detects, concentration and thermodynamics; sparation of bulk and grain boundary effects; polycrystalline Al_2O_3, pure and doped with Fe, Mg, Ti or Si.

UNIVERSITY OF SOUTHERN CALIFORNIA (Continued)

286. GRAIN BOUNDARY SLIDING DURING HIGH-TEMPERATURE CREEP — $69,500 — 01-02
T. G. Langdon - Materials Sciences and Mechanical Engineering Department

Experimental and analytical study of high temperature deformation of metals and ceramics; measurement of creep parameters-grain boundary sliding, activation energies, stress exponents; construction of creep deformation maps for parallel-and sequential-controlled deformation.

STANFORD RESEARCH INSTITUTE

287. CHEMISTRY OF ZIRCONIUM RELATED TO THE BEHAVIOR OF NUCLEAR REACTOR FUEL CLADDING — $134,952 — 03-03
D. Cubicciotti

Mass spectrometric measurement of the equilibria and thermodynamic constants of the interaction products of the zirconium-iodine system over a wide range of temperature conditions simulating a reactor environment; synthesis, enthalpy of formation, and heat capacity of ZrI_4; kinetics of iodide film formation and film characterization studies.

STANFORD UNIVERSITY

288. PHOTOVOLTAIC MATERIALS RESEARCH - II-VI HETEROJUNCTIONS AND Cu_2S/CdS THIN FILMS — $80,000 — 01-03
R. H. Bube - Materials Sciences and Engineering Department

Energy parameters and transport processes that control the electrical, photoelectronic and photovoltaic properties of the II-VI heterojunctions; preparation and control of reproducible properties between p-CdTe or p-ZnTe and n-CdSe, n-CdTe, n-ZnSe or n-ZnS; comparison of the properties of thin film and single crystal Cu_2S/CdS cells; effect of heat treatment, optical degradation, grain boundaries and temperature dependence.

STANFORD UNIVERSITY (Continued)

289. STRUCTURE DEPENDENCE OF HIGH TEMPERATURE DEFORMATION OF METALS — $60,000 — 01-02
W. D. Nix - Materials Sciences and Engineering Department

Experimental and theoretical project determining creep-rupture behavior in metal alloys; effect of gas bubbles on ductility and fracture; grain size effects; analysis of crack propagation and void coalescence at low strain rates.

290. DIFFUSION OF OXYGEN IN LIQUID METAL SYSTEMS — $35,938 — 01-03
D. A. Stevenson - Materials Sciences Department

Oxygen solubility, thermodynamic activity and diffusion in liquid metal alloy solutions; coulometric titration and time dependent currents using oxygen ion conducting solid electrolytes; Ga-In-O alloys.

UNIVERSITY OF TENNESSEE

291. MICROSTRUCTURE-PROPERTY RELATIONSHIPS IN AUSTENITIC STAINLESS STEELS — $26,000 — 01-01
J. E. Spruiell - Chemical and Metallurgical Engineering Department

Experimental study of effects of composition and initial ferrite content on microstructural stability of stainless steel weld metal; role of carbon content on sigma and chi phase precipitation in steels; recovery in steels of various stacking fault energies and pretreatment.

292. APPLICATION OF ADIABATIC CALORIMETRY TO METAL SYSTEMS — $37,000 — 01-03
E. E. Stansbury, C. R. Brooks - Chemical and Metallurgical Engineering Dept.

Heat capacity measurements of solid and liquid metals (Ga, Sn, Pb, Bi) near their melting point using solution calorimetry; heat effects associated with recovery and recrystallization of cold work stainless steel.

U. S. STEEL CORPORATION

293. STUDIES OF FUNDAMENTAL FACTORS CONTROLLING CATALYZATION OF REACTIONS OF GASES WITH CARBONACEOUS SOLIDS — $75,000 — 01-01
J. V. Mahoney - Research Laboratory

Experimental characterization of coal surfaces and catalytic activity at various stages of conversion of gaseous hydrocarbons; impurity and mineral effects; techniques used- high voltage and scanning electron microscopy.

UNIVERSITY OF UTAH

294. POSITRON LIFETIME MEASUREMENTS AS A NON-DESTRUCTIVE TECHNIQUE TO MONITOR FATIGUE DAMAGE — $48,677 — 01-02
J. G. Byrne, R. W. Ure, Jr. - Mechanical Engineering Department

Experimental study of microstructural defects generated during fatigue, strain aging, and hydrogen embrittlement of metals - Cu, Fe, Al, and their alloys; techniques used - positron annihilation, x-ray, transmission electron microscopy.

295. IMPURITY EFFECTS ON THE CREEP OF POLYCRYSTALLINE MAGNESIUM AND ALUMINUM OXIDES AT ELEVATED TEMPERATURES — $35,684 — 01-02
R. S. Gordon - Materials Sciences and Engineering Division

Determination of mechanisms of high temperature creep of polycrystalline oxide ceramics; role of impurities in determining roles of diffusional, grain boundary sliding, and dislocation mechanisms of creep; effects of impurities, temperature, oxygen pressure and grain size; MgO and Al_2O_3 doped with Fe, Cr and Mn-Ti; deformation maps.

VARIAN ASSOCIATES

296. RESEARCH ON LATTICE MISMATCHED SEMICONDUCTOR LAYERS — $70,000 — 01-03
R. L. Bell, G. A. Antypas - Solid State Laboratory

Fundamental investigations of growth and properties of solar photovoltaic heterojunctions, initially layered III-V compounds in the GaAs/InP system; minority carrier lifetimes; p-n junction characteristics; short circuit paths, epitaxial growth.

UNIVERSITY OF VERMONT

297. THERMODYNAMIC AND TRANSPORT PROPERTIES OF INTERSTITIAL HYDROGEN ISOTOPES IN METAL SYSTEMS — $21,518 — 02-03
J. S. Brown - Physics Department

Theoretical calculations of electronic and transport properties of liquid transition metals Pd and Ti, using Muffin-Tin potentials; electrical resistivity; thermopower; Hall coefficients; electron-phonon scattering and superconducting critical temperatures of Pd-H and Pd-D alloys.

UNIVERSITY OF VIRGINIA

298. ELECTRONIC PROPERTIES OF METALS AND ALLOYS, AND MOLECULES — $95,000 — 02-02
R. V. Coleman - Physics Department

Experimental and analytical investigation of electron and magnetic transport and band structure in ferromagnetic alloys (Fe and Co base); superconductivity, magnetoresistive properties, magnetic susceptibility, and Raman scattering of dichalcogenides (TaS_2, $TaSe_2$ and $NbSe_2$); electron tunneling spectroscopy of organic molecules; quantum interference effects in dilute metal alloys.

UNIVERSITY OF WASHINGTON

299. A STUDY OF PHASE TRANSFORMATIONS AND SUPERCONDUCTIVITY — $10,500 — 01-03
D. H. Polonis - Mining, Metallurgical and Ceramic Engineering Department

Relationship between phase transformations, microstructure and superconductivity in metal alloys; precipitation or transformation processes and powder metallurgical fabrication; effects of microstructure on Tc, H_{c1}, H_{c2} and hysteresis; β-stabilized, Zr-Nb alloys, Hf-Nb alloys, A-15 compounds dispersed in metal matrices.

UNIVERSITY OF WISCONSIN

300. VOID NUCLEATION AND GROWTH IN HEAVY ION AND ELECTRON BOMBARDED PURE METALS — $70,000 — 01-04
G. L. Kulcinski - Nuclear Engineering Department

Effects of irradiation variable and material parameters influencing void formation in metals; heavy ion and electron simulation of neutron irradiation; effects of temperature, fluence, flux and impurities; electron microscopy and swelling; high voltage electron microscopy; 18 MeV copper bombardment of V; 1MeV electron bombardment of Al.

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.

SUMMARY OF
FUNDING LEVELS

During the fiscal year ending June 30, 1976, the Materials Sciences total support level amounted to about $43.9 million in operating funds and $3.0 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. The next fiscal year begins October 1, 1976. This report also includes some of the new programs started in the transition period July 1, 1976 - September 30, 1976.

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.)	41.5	16.3
(b) South ..... (Fla., N.C., Tenn., Va., Georgia)	6.9	25.0
(c) Midwest ..... (Ohio, Ill., Wisc., Mich., Minn., Ind., Iowa, Kan.)	23.0	41.4
(d) West ..... (Ariz., Okla., Wash., Texas, Hawaii, N. Mex., Calif., Utah, Col., Idaho)	28.6	17.3
	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-)	60.5	43.5

	Contract Research (%)	Total Program (%)
(b) Physics, Solid State Science, Solid State Physics (Office Budget Activity Numbers 02-)	33.2	41.0
(c) Chemistry, Chemical Eng. (Office Budget Activity Numbers 03-)	6.3	15.7
	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)	35.9
(b) Laboratory Program	64.1
	100.0

4. By Laboratory:

	Total Program (%)
Ames Laboratory	10.5
Argonne National Laboratory	24.3
Brookhaven National Laboratory	10.7
Idaho National Engineering Laboratory	0.1
Illinois, University of (Materials Research Laboratory)	3.5
Lawrence Berkeley Laboratory	8.9
Lawrence Livermore Laboratory	0.7
Los Alamos Scientific Laboratory	1.4
Mound Laboratory	0.3
Oak Ridge National Laboratory	24.2
Pacific Northwest Laboratory	1.9
Sandia Laboratory	0.5
Contract Research	13.0
	100.0

5. By Selected Areas of Research:

	Number of Projects (Total=267) (%)	Total Program $ (%)
(a) Materials		
Actinide Metals and Compounds	8.2	6.8
BCC Refractory Metals	15.0	7.0
Ceramics	24.0	13.8
Rare Earth Metals and Compounds	9.0	6.5
Liquids	10.5	5.7
Semiconductors	11.6	5.1
(b) Technique		
Neutron Scattering	7.5	16.3
Theory	7.5	5.9
(c) Phenomena		
Catalysis	4.1	3.4
Corrosion	5.6	2.0
Diffusion	12.4	5.6
Superconductivity	12.0	9.9
Strength	17.2	11.1
Surface Phenomena & Thin Films	15.7	11.4
(d) Environment		
Hydrogen	9.4	4.7
Radiation	13.1	17.4

SECTION D

Index of Investigators, Materials, Phenomena, Technique and Environment

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

Actinide Metals and Compounds

1	128
4	129
24	130
25	132
26	133
44	134
45	135
53	140
54	146
58	155
117	161

Ceramics

Carbides	Glass	Nitrides	Oxides			
3	24	50	2	48	122	230
50	37	53	3	50	129	246
51	43	134	9	53	130	251
53	104	163	22	54	132	252
54	123	246	25	56	134	255
78	156	258	27	64	135	258
85	214		29	66	141	271
129	218		31	70	143	275
146	236		35	74	146	276
258	278		37	86	156	280
			39	88	201	285
			40	104	202	286
			46	106	216	295

Composites

3	129
8	130
83	134
103	213
107	235

Fast Ion Conductors

12	91
14	97
31	141
38	146
46	153
59	212
66	271
71	

Graphite, Carbon, and Coal

15	129
19	210
58	218
107	269
120	277
121	293

Hydrides

2	46
7	51
9	81
25	82
31	140
32	206
38	243
44	247

Intermetallic Compounds

5	37	61	142
7	41	62	149
8	44	67	159
10	45	74	160
24	49	103	210
		136	219

Ionic Crystals

10	70	138
11	72	143
16	73	218
37	74	246
39	91	248
40	123	268
		298

Liquids & Amorphous Metals

3	46	75	151
12	49	77	152
18	55	97	153
37	56	109	205
41	60	114	223
43	69	127	224
	71	128	263
			290

Metals

Alkali

15
55
127
223
224
269

BCC Refractory

1	55	162	247
2	80	164	253
4	81	216	261
8	82	220	265
9	85	227	267
16	87	231	270
17	133	237	274
31	135	239	282
34	143	242	289
50	147	245	300

Ferrous

1	134	223	270
10	135	225	273
34	137	231	274
76	159	233	279
98	203	234	281
99	204	237	283
100	215	240	291
101	216	261	292
102	217	262	

MHD Materials

2
25
27
38
39
48
53

Organics

7	87
15	89
40	112
47	140
51	151
52	164
58	235
60	246
64	284

Rare Earth Metals and Compounds

1	49
3	51
5	53
6	54
9	58
11	138
14	139
16	146
18	201
32	205
37	243
44	250

Semiconductor

3	39	108	145	228
5	47	110	146	236
9	49	112	156	241
10	52	130	157	249
12	54	138	163	264
23	102	143	218	288
				296

Acoustic Emission

84
262

Auger Spectroscopy

23
28
68
122
144
229
261

Computer Simulation

29
43
71
208
254
258

Elastic Constants

3
31
245

Electron Microscopy

4	57	133	215	231	264
29	82	137	216	241	270
30	98	148	220	242	293
31	102	202	228	243	300
33	126	203	229	253	
35	129	207	230	258	

Electron Spin Resonance

40
43
141
212

Field Ion Microscopy

23
50
164
237

High Temperature Heat Capacity

18
135
292

Infrared Spectroscopy

57
108
111
124
141

Internal Friction

29
78
81
90
215
267

Laser Beam Scattering

109
117
123
158
218
222
257
271

Low Temperature Specific Heat

24
41
53
61
114
135
249
263

Magnetic Susceptibility

3
6
24
26
44
76
203

Neutron Scattering

5 66
15 69
25 138
27 139
37 140
38 151
51 201
63 247
64 256
65 259

Nuclear Magnetic Resonance

7
24
43
77
87
93
121
206
212

Optical Spectroscopy

10
46
96
110
123
141
145
158
163
268
275
278

Positron Annihilation

31
73
267
294

Sputtering

9
42
52
80
118
157
159
160
161

Synchrotron Radiation

10
70
132
266

Theory

1	209
12	213
13	214
14	221
49	232
71	233
112	235
127.5	238
131	258
146	297

Thermal Conductivity

3
97
128
135

Thermodynamics

1
3
9
54
55
56
58
105
116
129
153
224
287

X-Ray Photoelectron Spectroscopy

22
24
28
52
122
144

X-Ray Scattering

3	92
15	132
25	148
29	151
51	201
52	245
54	247
57	278

Catalysis

23 120
28 144
43 151
68 154
88 293
93

Channeling

33
73
144
149
163

Corrosion

55 159
75 202
79 216
84 223
101 225
117 272
122 274
155

Crystal Structure, Atomic Distribution and Crystal Transformations

1 124
3 127.5
5 128
15 129
22 161
25 201
27 203
28 230
43 232
51 243
64 278
98 299

Diffusion

1	91	229
2	104	231
3	105	255
21	127	256
31	134	258
36	152	271
37	153	279
54	156	284
55	165	285
81	212	290
87	214	297

Dislocations

29
90
102
131
226
241
254

Erosion

30
101
129
133

Electron Transport

1	113
3	125
9	128
26	135
27	141
45	147
48	156
62	205
86	220
89	238
96	298
106	

Electronic Structure

Magnetism

Materials Preparation and Characterization

Phonons

Photovoltaic and Photothermal Phenomena

Point Defects

Precipitation

Recovery and Recrystallization

Sintering

Solidification

Strength

Fracture

2 231
81 242
82 261
84 262
101 283
204 289

Fatigue

29
223
282
294

Creep

29 234
126 235
137 251
161 258
162 284
220 285
233 286
289

Flow Stress

2 129 240
4 133 242
29 161 253
78 165 254
83 204 267
85 215 270
100 220 276
101 233 277
234 295

Stress-Corrosion Cracking

84
155
217
261
274
281

Superconductivity

3 49 111 210
7 61 112 219
8 62 136 238
13 67 140 239
32 73 142 244
34 95 160 246
38 97 205 249
42 103 209 263

Surface Phenomena and Thin Films

1 33 67 118 144 164
3 35 68 120 149 222
8 42 75 123 150 223
10 47 79 125 152 229
12 49 88 130 154 246
23 50 97 134 155 264
28 52 104 135 158 287

Gas

Oxidizing	Hydrogen			Sulphur-Containing
1	1	38	140	3
80	2	46	165	57
87	7	51	206	134
122	9	55	231	
134	25	81	243	
159	31	82	247	
290	32	127	273	
	37	133	282	
		135	284	

Magnetic Field

3	44
5	45
6	63
7	76
8	93
24	103
25	121
37	139

Pressure

Above Atmospheric
9
37
65
89
92
113
245
251

Radiation

Electron	Ion		Neutron		Photons	Theory	Gamma
33	4	137	4	148	123	72	40
35	33	148	34	150	158	94	73
50	34	149	50	162		146	248
72	35	150	62	203		221	
94	36	162	72	220			
137	50	207	126	253			
216	62	237	137	277			
270	73	249	147				
	102	258					
	126	300					

Temperature

Very Low Temperatures

8	114
9	124
26	211
41	244
53	249
69	260
97	263

High Temperatures

1	105
16	116
18	125
22	130
27	135
52	224
54	250
60	269
101	