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Materials Sciences Programs

Fiscal Year 1981

Office of Basic Energy Sciences

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

September 1981

FOREWORD

The Division of Materials Sciences is located within the Department of Energy in the Office of Basic Energy Sciences. The organizational structure of the Department of Energy is given in an accompanying chart. The Office of Basic Energy Sciences reports to the Director of the DOE Office of Energy Research. The Director of this Office is appointed by the President with Senate consent. The Director advises the Secretary on the physical research program; monitors the Department's R&D programs; advises the Secretary on management of the multipurpose laboratories under the jurisdiction of the Department excluding laboratories that constitute part of the nuclear weapon complex; and advises the Secretary on basic and applied research activities of the Department.

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

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

This report contains a listing of all research underway in FY 1981 together with a convenient index to the program.

Donald K. Stevens, Director
Division of Materials Sciences
Office of Basic Energy Sciences

INTRODUCTION

The purpose of this report is to provide a convenient compilation and index of the DOE Materials Sciences Division programs. This compilation is intended for use by administrators, managers, and scientists to help coordinate research and as an aid in selecting new programs.

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

Each project carries a number (underlined) for reference purposes. The FY 1980 funding level, title, personnel, budget activity number (e.g., 01-2), and key words and phrases accompany the project number. The first two digits of the budget number refer to either Metallurgy and Ceramics (01), Solid State Physics (02), or Materials Chemistry (03). The budget numbers carry the following titles:

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

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

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

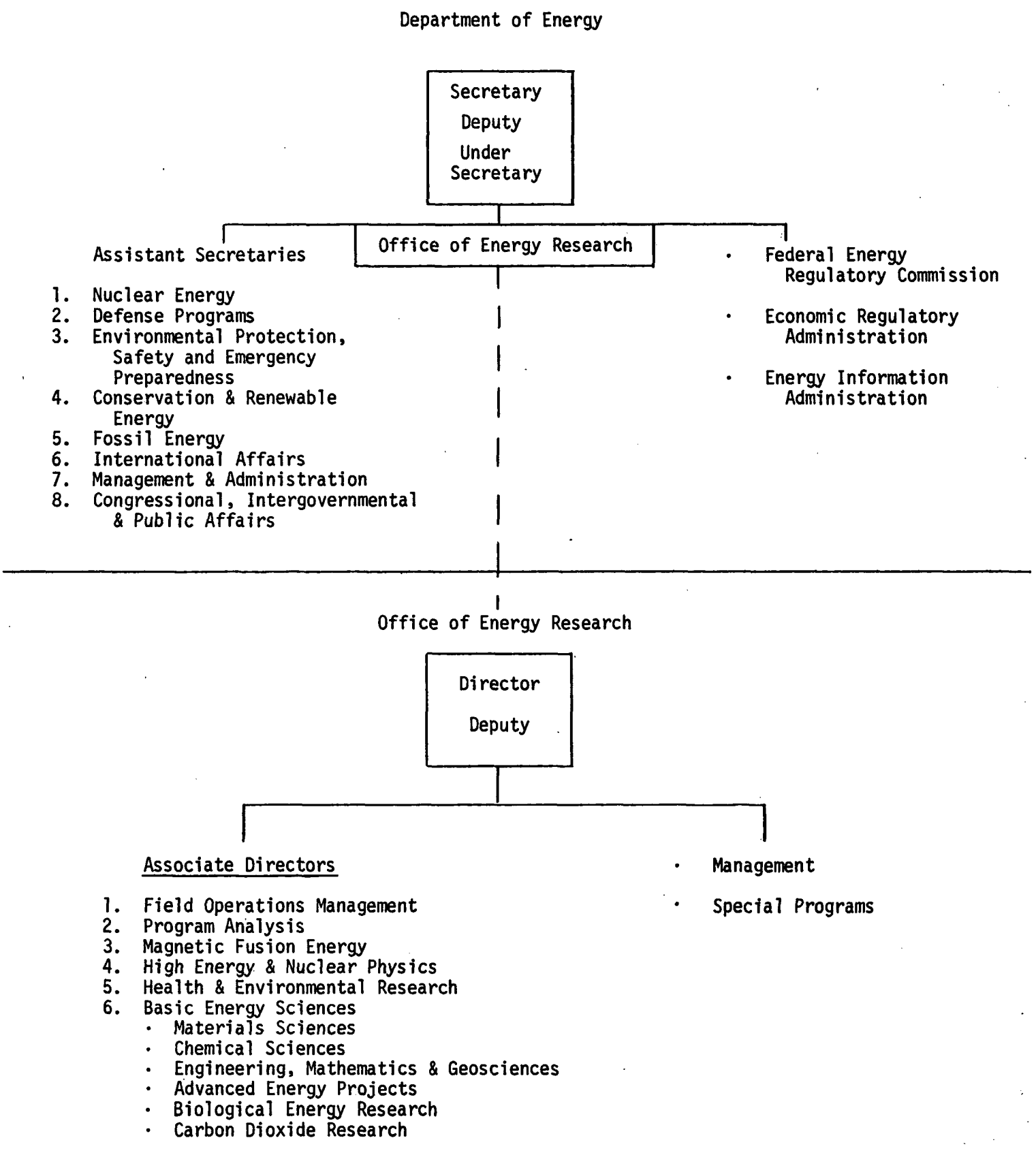
Section C summarizes the total funding level in a number of selected categories. Obviously most projects can be classified under more than one category and, therefore, it should be remembered that the categories are not mutually exclusive.

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

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

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

ORGANIZATION OF THE DEPARTMENT OF ENERGY

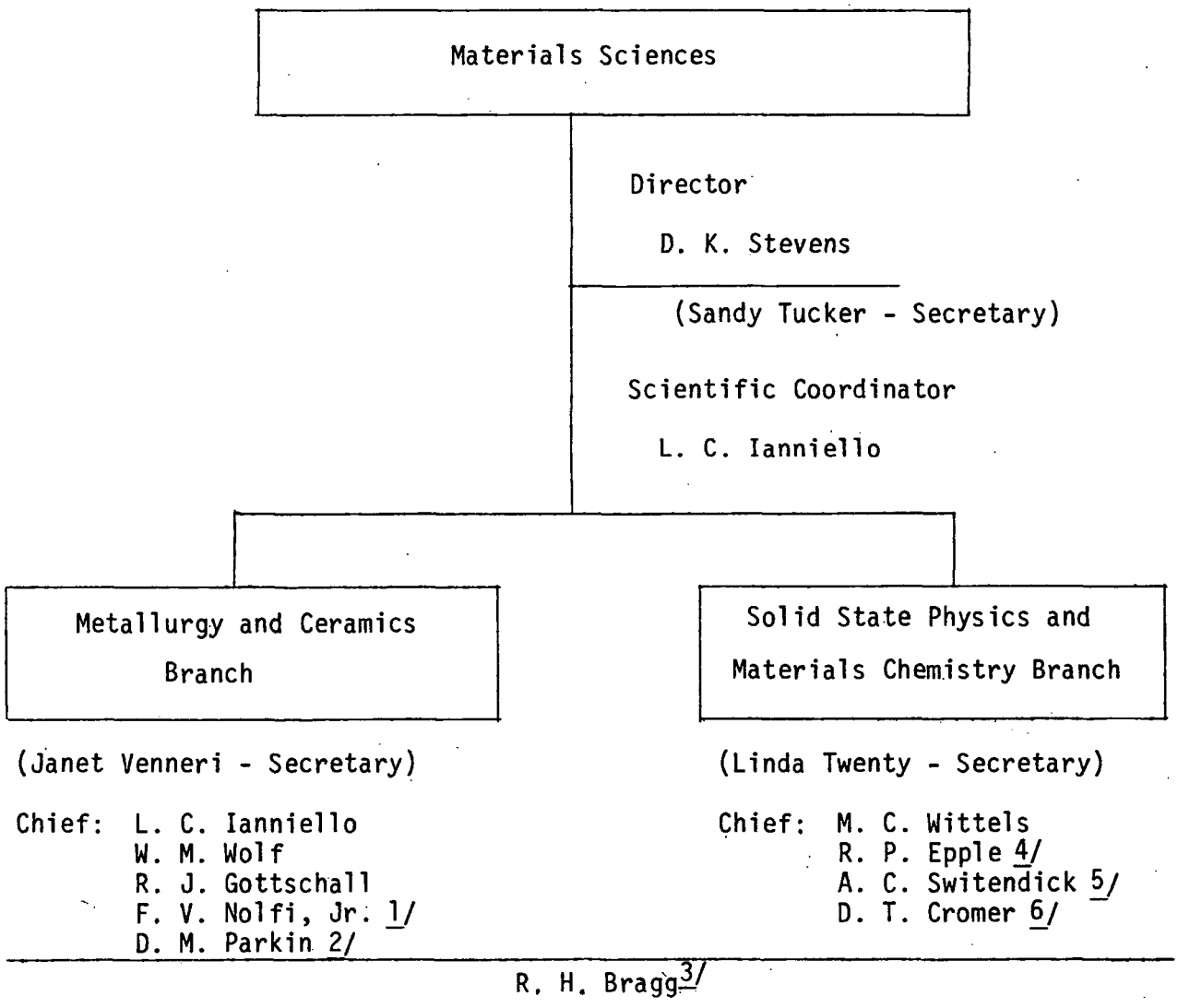


STRUCTURE

OF THE

DIVISION OF MATERIALS SCIENCES

OFFICE OF BASIC ENERGY SCIENCES



Notes:
1/ Reporting to Ames Laboratory 8/81
2/ On Leave from Los Alamos National Laboratory
3/ On Leave from Lawrence Berkeley Laboratory
4/ Retired 8/81
5/ On Leave from Sandia National Laboratories - Albuquerque
6/ On Leave from Los Alamos National Laboratory

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SECTION A

Laboratories

This information was provided by the Laboratories. Most projects are of a continuing nature although specific projects were concluded in FY 1981.

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

Metallurgy and Ceramics -01-
F. V. Nolfi - Phone: (FTS) 865-4446 or 515-294-4446

1. CONTROLLED MICROSTRUCTURES — $260,000 — 01-1
R. K. Trivedi, J. D. Verhoeven, E. D. Gibson, J. T. Mason, F. Laabs

Theoretical studies of the effect of temperature gradient, growth rate, and composition on the characteristics of dendritic interfaces obtained during controlled solidification. Study of morphological transitions from cellular to dendritic to eutectic structure. Experimental work on dendritic growth in Pb-Sn and Pb-Au alloys by using a controlled solidification technique. Study of morphological development in prototype transparent materials such as succinonitrile and Borneol. Preparation of composite Cu-Fe alloys by an *in situ* casting/mechanical reduction technique and evaluation of structure dependence of resistivity/strength ratio. A study of directionally transformed pearlite at off-eutectoid compositions. Fabrication of Nb_3Sn-Cu superconducting composite wire by the *in situ* process: casting and mechanical reduction to wire of Nb-Cu alloys followed by Sn diffusion. Optimization of J_c properties by control of microstructure and alloy additions. Development of arc casting techniques for scale-up. Study of factors affecting the reliability of the Sn diffusion process.

2. MASS TRANSPORT IN SOLIDS — $ 89,000 — 01-1
O. N. Carlson, F. A. Schmidt

Measurement of fast diffusion and electrotransport behavior of metallic solutes in yttrium, scandium and thorium. Use of internal friction to characterize defects associated with fast transport process. Thermotransport of interstitial solutes in ferrous and refractory metal alloys. Transport of carbon in two phase Nb-C, Fe-Ni-C and V-Ti-C alloys in presence of temperature gradient. Development and testing of model to explain mass transport in two-phase alloys.

3. SOLAR MATERIALS AND SYSTEMS — $124,000 — 01-1
B. J. Beaudry, K. A. Gschneidner, Jr., F. A. Schmidt, R. K. Trivedi

Determination of the Schottky barrier heights of rare earth metal-silicon systems; heteroepitaxial growth of silicon on inexpensive substrates such as metal silicides and Fe-3 wt% Si. High temperature electric mobility and diffusivity of metallic solutes in silicon. Precipitation of primary grains of silicon from pure metals and from off-eutectic liquid alloys. Preparation of rare earth sulfides near the composition $RS_{1.50}$ for photovoltaic conversion devices; low temperature heat capacity measurements and characterization studies of polycrystalline R_2S_3 phases.

4. EMBRITTLEMENT OF FERRITIC ALLOYS $ 56,000 01-1
O. N. Carlson

Effect of alloy composition and residual impurities on strength and bend ductility of 9 Cr-1 Mo ferritic alloy in quenched, tempered, and 450°C-aged conditions. Comparison of smooth and notched slow bend test results.

5. RARE EARTH AND OTHER METAL PREPARATION $211,000 01-1
B. J. Beaudry, O. N. Carlson,
K. A. Gschneidner, Jr., F. A. Schmidt

Preparation of high purity rare earth and vanadium metals from their oxides for use in various basic and applied research projects at Ames Laboratory, other DOE Laboratories, and other institutions; metallothermic reduction processes are used. Ultrapurification of rare earth, zirconium and vanadium metals by electrotransport and by zone melting processes.

6. HYDROGEN IN REFRACTORY METALS AND HYDROGEN ATTACK $156,000 01-2
O. Buck, C. V. Owen

Characterization of deformation modes, hydrogen precipitation and crack initiation in refractory metals and alloys using electron microscopy; measurements of the acoustic emission generated by hydride formation with and without applied stress. Internal friction studies in hydrogen doped refractories. Effects of methane bubble formation, due to hydrogen attack, on creep, fatigue and strength of steels.

7. FRACTURE MECHANICS AND STRESS CORROSION $145,000 01-2
O. Buck

Growth of fatigue cracks in steels exposed to harsh environments with major emphasis on steels in H_2, H_2S, etc.; the effects of fracture mode changes in such environments on the scattering of acoustic waves. Development of new nondestructive evaluation techniques and the determination of their applicability. Microscopic characterization and modeling of microcrack initiation under stress corrosion conditions.

8. MECHANICAL PROPERTIES OF CERAMICS $ 80,000 01-2
O. Hunter

Studies of transformation toughened Al_2O_3-ZrO_2/HfO_2 and related microcracking during thermal cycling from room temperature to 1500°C. Creep of Y_2O_3.

9. MARTENSITIC TRANSFORMATIONS IN SHAPE MEMORY ALLOYS AND CERAMICS — $ 91,000 — 01-2
M. S. Wechsler

Resistivity and strain measurements in Ni-Ti during temperature cycling above and below the martensitic transformation under various loading conditions are used to relate the transformation behavior to the applied stress state. Applications considered are: (1) use of shape memory alloys in low-temperature heat engines, and (2) transformation toughening in ceramics, particularly ZrO_2 and HfO_2.

10. RARE EARTH ADDITIONS TO STEELS — $ 48,000 — 01-2
M. S. Wechsler

The effects of rare earth additions on the elevated temperature mechanical properties, irradiation-swelling behavior, electron microscopy, and metallography of austenitic and ferritic steels. Uniaxial tensile and indentation hardness tests. Rare earth additives are Y, Ce, and La in concentrations below one percent.

11. THERMODYNAMICS, PHASE EQUILIBRIA, AND ALLOY THEORY — $ 89,000 — 01-3
J. F. Smith, D. M. Bailey,
K. A. Gschneidner, Jr.

Development of thermodynamic functions describing alloy formation in refractory metal alloys and lithium alloys through vapor pressure and EMF techniques. Computer analysis of consistency between thermodynamic and phase equilibria data. Data analysis for vanadium and niobium systems. Statistical analysis and predictability of terminal solubilities in binary alloys.

12. ULTRASONIC MEASUREMENTS — $ 74,000 — 01-3
J. F. Smith, J. D. Greiner

Elastic constants at low temperatures of single crystals of lutetium with dilute concentrations of hydrogen to test for electronic effects. Elastic constants at elevated temperatures of single crystals of yttria-stabilized zirconia as functions of both temperature and composition to correlate with the martensitic transformation in zirconia. Tests on single- and poly-crystals of aluminum in stressed states to develop criteria and techniques for the ultrasonic determination of residual stress.

13. DIFFUSION IN CERAMICS — $142,000 — 01-3
M. F. Berard, C. D. Wirkus

Studies of cation self-diffusion, interdiffusion, electrical conductivity, defect structure and phase equilibrium relationships in fluorite structure binary and ternary alloys based on HfO_2 and ZrO_2, and in pure and doped rare-earth oxides.

14. SULFIDATION $ 51,000 01-3
C. W. Chen

Mechanisms and kinetics of early-stage sulfidation of iron and iron-chromium alloys; use of surface sensitive techniques such as ESCA, Auger spectroscopy, and electron microscopy. Effect of oxide layers on initiation of sulfidation.

15. AMORPHOUS MAGNETIC MATERIALS $ 29,000 01-3
C. W. Chen

Fabrication by splat cooling of amorphous ribbons of $Fe_{82}B_{18-x}Be_x$ and $Fe_{82}B_{18-x}Au_x$. Magnetic properties, electronic structure, and crystallization of these ribbons. Magnetic moment of Fe in these alloys.

16. HYDROGEN IN METALS $197,000 01-3
D. T. Peterson

Diffusion, thermotransport, partial molar volume and solubility of H and D in V alloys with Ti, Cr or Nb. Photoelectron spectroscopy, optical properties and metallography of metal hydrides.

17. TRANSFORMATION STUDIES AND ORDERED ALLOYS $ 77,000 01-3
F. X. Kayser

Temperature dependence of the elastic constants of single crystals of γ' phase materials including Ni_3Al and alloys in the system Ni_3Al:Ni_3Ti. High-strain rate co-axial extrusion and cladding of high-silicon irons with steel; relationship between extrudability and structure of the silicon-iron. Corrosion resistance of carbon-free high-silicon irons.

18. SUPERCONDUCTIVITY AND LOW TEMPERATURE PHENOMENA $241,000 01-3
K. A. Gschneidner, Jr., O. D. McMasters,
B. J. Beaudry

Preparation and measurement of the superconducting transition temperatures of La_3S_4-La_3Se_4 and $(La_{3-x}M_x)S_4$ alloys with M = Mg, Ce, Y, Th. Low temperature (1-20K), high magnetic field (0-10T) heat capacity study of lattice instability, electron concentration and size effects in rare-earth based superconductors: La_3S_4-La_2S_3, La_3S_4-La_2Se_3, and $(La_{1-x}R_x)(In_{1-y}M_y)$ with R = Sc, Y, Lu and M = Sn, Cd. Low temperature (1-20K) - high magnetic field (0-10T) heat capacity study of spin fluctuations and magnetic phenomena in (1) highly enhanced paramagnets: $CeSn_3$, RCo_2 (R = Sc, Y and Lu), $Pd_{1-x}Ni_x$ (x = 0.5 and 1.0), and Sc; and (2) itinerant ferromagnets: Sc_3In and $ZrZn_2$.

19. CERAMIC PROCESSING $180,000 01-5
M. Berard, O. Hunter, M. Akinc

Studies of the influence of preparation procedures on characteristics of precursor precipitates (yttrium hydroxide, carbonate, oxalate) and resulting Y_2O_3 powders. Acetone-toluene-acetone dewatering. Controlled humidity drying. Powder morphology, surface characteristics, sinterability.

20. NON-DESTRUCTIVE EVALUATION $220,000 01-5
C. P. Burger, L. W. Schmerr,
D. O. Thompson, L. W. Zachary,
W. J. Higby

Dynamic photoelastic visualization combined with ultrasonic Rayleigh surface wave techniques for measuring the depth of surface-breaking cracks. Crack modeling of zero volume cracks based on boundary integral equation techniques. Flaw identification using a frequency domain algorithm to obtain the complex resonance of a flaw. Applications of the displacement discontinuity method in two-dimensions to determine the stress concentration factor for an elliptical void near a boundary, and the stress intensity factor for an angled surface breaking crack in a plate. Ultrasonic scattering measurements to characterize pores and multiple voids in glass; velocity and attenuation of ultrasonic waves in glass.

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

21. NEUTRON SCATTERING $330,000 02-1
W. A. Kamitakahara, C. Loong,
C. Stassis, J. Zarestky

Study of the lattice dynamics, thermodynamic properties and structural transformations of metals at high temperatures (Zr, Re, La, Tc); structure and diffusion in metal hydrides (ScH_x, LaH_x); dynamics and phase transitions of alkali-graphite intercalation compounds; electronic structure and phonon spectra of mixed valence compounds ($CeSn_3$, $CeIn_3$, $CePd_3$); relation of electron-phonon interaction to superconductivity (La, $LaSn_3$).

22. SEMICONDUCTOR PHYSICS $230,000 02-2
A. J. Bevolo, H. R. Shanks,
F. Jeffrey

Preparation and characterization of r.f. sputtered hydrogenated amorphous silicon and Schottky barriers; measurement of gap states. Growth and characterization of single crystal tungsten bronzes (H_xWO_3, Na_xWO_3, Rb_xWO_3) and layer structure semiconductors (WSe_2, $ZrSe_2$, $MoSe_2$); electrical resistivity, Hall effect, photoemission. Auger, ELS, and SIMS studies of surfaces and interfaces: metal-semiconductor interfaces (Si on transition metals, rare earths on silicon), Fe-B based amorphous alloys, tin and its oxides, sulfidation of iron-based alloys, corrosion inhibitors on copper, oxygen role in redox reactions on platinum electrodes, and diffusion in ceramics.

23. SUPERCONDUCTIVITY $360,000 02-2
D. K. Finnemore, J. R. Ostenson,
E. L. Wolf, T. P. Chen, S. Nagata,
T. Refai

Electron tunneling spectroscopy and surface physics studies of strong-coupled transition metal superconductors, including alloys and compounds. Conventional and proximity electron tunneling spectroscopy (PETS) of the electron-phonon spectrum $\alpha^2F(\omega)$. Auger electron spectroscopy (AES), electron energy loss spectroscopy (ELS) and ultraviolet photoemission spectroscopy (UPS). Fundamental studies of superconductivity in inhomogeneous materials; supercurrents in normal metals near a superconductor normal metal boundary; development of superconducting composites suitable for large scale magnets in the 8 to 14 Tesla range; practical studies to improve wire fabrication techniques and performance characteristics such as critical currents and ac losses.

 Lynch -

24. OPTICAL AND SPECTROSCOPIC PROPERTIES OF SOLIDS AND LIQUIDS — $310,000 — 02-2

F. S. Khumalo, D. W. Lynch, C. G. Olson, M. Piacentini, F. H. Spedding, J. Kester, D. L. Rath

Electron photoemission and optical properties (transmission, reflection, EXAFS, thermoreflection, thermotransmission, electroreflection) of solids in the near infrared, visible vacuum ultraviolet and soft X-ray region (using synchrotron radiation): transition metal alloys and compounds (e.g., Nb_xMo_{1-x}), transition metal-hydrogen systems, layered transition metal chalcogenides ($MoSe_2$), amorphous metals. Photoemission into liquid electrolytes, electrochemical modulation spectroscopy, surface Raman scattering, and photoelectrochemistry on binary alloys susceptible to localized corrosion (benzotriazole on Cu). Surface excitation, and adsorption phenomena on model systems (e.g., noble metals). Photoelectrolysis employing layered compounds. Crystal field and Zeeman spectra of rare earth ions in crystals.

25. NEW MATERIALS AND PHASES — $420,000 — 02-2

R. N. Shelton, C. A. Swenson, M. S. Anderson, R. G. Barnes, D. R. Torgeson, F. Borsa, M. L. S. Garcia

Synthesis and characterization of new ternary compounds such as Chevrel phases, ternary transition metal borides and rare earth transition metal silicides. Study of the physical properties of these new materials, such as microhardness, phase equilibria and their refractory nature, and high temperature behavior. Properties of new ternary phases at low temperatures, including magnetic susceptibility, transport properties, heat capacity, coexistence of superconductivity and long range magnetic order. High pressure equations of state of new materials, elementary solids (alkali and alkaline earth metals); effects of hardness on thermal expansivities of technical materials (beryllium copper); low temperature expansivity of materials (Lu) containing hydrogen. Applications of NMR to hydrogen embrittlement of refractory metals (V, Nb, Ta) and alloys (V-Ti, Nb-V), trapping of hydrogen by interstitial impurities in these metals, structural and electronic characterization of hydrogenated amorphous silicon films.

26. MATERIALS FOR HYDROGEN STORAGE $160,000 02-2
R. G. Barnes, J. D. Corbett, K. A. Gschneidner, Jr., B. N. Harmon, W. A. Kamitakahara, D. T. Peterson, T. Ito, H. Marek, C. K. Saw, R. Schoenberger

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

27. X-RAY DIFFRACTION PHYSICS $100,000 02-2
J.-L. Staudenmann

X-ray diffraction studies of martensitic phase transitions (V_3Si and Fe-C) and electron charge densities; small angle scattering, EXAFS, microdiffraction. Studies of electron density near interstitial impurities. MATRIX PRT beam line at NSLS.

28. ELECTRONIC AND MAGNETIC PROPERTIES $300,000 02-3
B. N. Harmon, K.-M. Ho, R. A. Klemm, S. H. Liu, D. Misemer, M. Nolan, S. Gadekar

Theory of phonon anomalies, lattice instabilities and soft modes in metals and their relation to the electron-phonon interaction and superconductivity (Nb, Mo, Zr, Ti). Surface electronic structure of metal electrodes (e.g., Ag), electroreflectance, and microscopic properties of the metal-electrolyte interface. Static and dynamic properties of mixed valence compounds ($CeSn_3$). Electronic properties and chemical bonding of transition and rare earth metal compounds (ZrB_2, $ZrSe_3$, ZrS, TiS, PtTe). Renormalization group studies of phase transitions.

29. OPTICAL AND SURFACE PHYSICS THEORY $ 80,000 02-3
R. Fuchs, K. L. Kliewer

Optical properties of metals, semiconductors, and insulators; studies of surfaces, thin films, layered systems, small particles, and powders. Differential surface reflectance spectroscope. Raman scattering from molecules adsorbed on metal surfaces. Photoemission and electroreflectance with emphasis on surface states. Photoemission into liquid electrolytes and related catalytic, electrochemical, adsorption, and corrosion effects; anodic photocurrents; the liquid metal interface. Solar energy studies: electrochemical photovoltaic cells, photolysis, high-temperature adsorbers, and optical properties of phase-change materials for solar applications.

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

Electrodynamics of superconductor-normal metal composites. Properties of current-carrying type-I and type-II superconductors containing magnetic flux; induced voltages and energy dissipation due to flux motion; flux-flow voltage noise; vortex nucleation and surface pinning; behavior of arrays of nonparallel vortices; critical currents and flux pinning in inhomogeneous superconductors; instabilities; ac losses; superconductivity and magnetic ordering in ternary rare earth compounds (Chevrel phases); the influence of reduced dimensionality on the superconducting properties of highly anisotropic systems; new mechanisms for superconductivity in linear conductors; triplet superconductivity and its physical properties.

Materials Chemistry Division -03-
L. E. Burkhart - Phone: (FTS) 865-8074 or 515-294-8074

31. X-RAY AND NEUTRON CRYSTALLOGRAPHY $189,000 03-1
R. A. Jacobson, B. J. Helland, D. M. Bailey

Development of diffraction techniques for single crystal and non-single crystal specimens; indirect methods and refinement techniques; operation of X-ray characterization facility; radial distribution function analysis of amorphous scattering from coal; structural studies of intramolecular solid state interactions which modify properties of parent species; metal complex structures with emphasis on model homogeneous catalysts and polymetal species.

32. METAL-METAL BONDING IN SOLID STATE MATERIALS $176,000 03-1
J. D. Corbett, R. C. Burns

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

33. CHEMISTRY OF HEAVY TRANSITION METALS $155,000 03-1
R. E. McCarley, L. Brough

Chemistry of heavy transition elements, especially Nb, Ta, Mo, and W; controlled synthesis and characterization of compounds with strong metal-metal bonds in dimers, clusters, and extended structures; relation of molecular and electronic structure of such compounds to electrical and thermal conductivity, mechanical strength, catalytic properties, chemical reactivity, and superconductivity; condensation reactions of metal cluster compounds.

34. METALS FROM FLY ASH $165,000 03-2
G. Burnet, M. J. Murtha, J. W. Dunker

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

35. PARTICULATE PROCESSING $270,000 03-2
L. E. Burkhart, A. Cahill, K. S. Chou

Transport near interfaces, especially drops, bubbles, and solid particles; kinetics and control of particle size distribution, growth rate, and morphology in both liquid phase and vapor phase operations involving the preparation of ceramic powders (yttria, urania, titania); reaction kinetics and mixing in multicomponent mass transfer systems involving chemical reactions with emphasis on correlation between theory and experiment (metal recovery processes).

36. HIGH TEMPERATURE CHEMISTRY $223,000 03-3
H. F. Franzen, R. A. Schiffman,
I. Shilo

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

37. SURFACE CHEMISTRY AND CATALYSIS $297,000 03-3
R. S. Hansen, B. A. Parkinson,
K. G. Baikerikar, D. C. Johnson

Heterogeneous catalysis, reactions at clean surfaces associated with coal liquefaction and gasification (e.g., methanation reaction on ruthenium and hydrodesulfurization using non-stoichiometric rare earth sulfides); field emission, flash desorption, LEED and Auger spectroscopy techniques for studying reaction kinetics and composition of surface phases resulting from the interaction of gases such as CO and H_2 on catalyst single crystal faces; electrical double layer properties and their alteration by adsorption; electrocatalysis at binary electrode surfaces for control of toxic or mutagenic organic molecules (nitrosoamines, polynuclear compounds) in wastes; preparation and electrochemistry of layered chalcogenide photochemical converters (e.g., MoS_2, $MoSe_2$, WSe_2).

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

Materials Science Division - 01-

B. R. T. Frost - Phone (FTS) 972-4928 or 312-972-4928
F. Y. Fradin - Phone (FTS) 972-4925 or 312-972-4925

38. ALLOY PROPERTIES $742,000 01-1
D. J. Lam, A. T. Aldred, A. J. Arko, S. K. Chan, G. S. Knapp, B. W. Veal, K. I. Kumagai

Experimental and theoretical studies of electronic structure and its relationship to physical and chemical properties and bonding in solids; XPS and EXAFS studies of the structural and electronic properties of various metal oxides in sodium silicate glasses; crystal chemistry and structural stability of complex transition metal oxides; x-ray absorption near-edge spectroscopy (XANES) study of 3d-ion coordination in complex oxides; formulation of the theory of EXAFS and XANES taking into account multiple scattering, interstitial potential, and lattice vibrations; theoretical studies of charge density, bonding and photoemission in transition-metal and actinide compounds using self-consistent relativistic molecular cluster calculations; dHvA, ARPES, XPS, UPS, NMR, and magnetization studies of actinide metals and intermetallic compounds to determine band structure, electronic configuration and stability of 5f electron states.

39. SCATTERING STUDIES $510,000 01-1
M. H. Mueller, J. E. Epperson, J. Faber, G. H. Lander

Magnetic, electronic, and structural properties of actinide materials using neutron scattering; particular emphasis on measurements on single crystals using both elastic and inelastic neutron scattering; studies of anharmonicity and covalent bonding effects in intermetallic AB_3 compounds and ABO_4 compounds as crystalline solids for waste storage use; structural investigations of metal hydrides of the type ZrNiD; x-ray diffuse and neutron small-angle scattering experiments of alloy decomposition, e.g., in α-Ni-Al; small-angle x-ray scattering investigation of voids formed in oxygen doped Nb. Major involvement with design, construction, and operation at the Argonne Intense Pulsed Neutron Source; group is responsible for small-angle neutron scattering prototype and for the general purpose powder diffractometer at IPNS and has major interest in the single crystal instrument for elastic scattering studies, and time-of-flight chopper spectrometers for inelastic studies; development of x-ray diffuse scattering instrumentation for midwest-materials science participating research team at the National Synchrotron Light Source.

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

40. SURFACE STUDIES — $265,000 — 01-1
M. B. Brodsky, S. D. Bader,
L. Richter

Electronic and atomic structure of intermetallic compound and transition metal surfaces; surface magnetism; thermal desorption of gases from Ru-Cu overlayers; electronic structure modifications in thin epitaxial metal sandwiches; low energy electron diffraction, x-ray and ultraviolet photoelectron spectroscopy; electron loss spectroscopy; Auger electron spectroscopy.

41. STRENGTH AND DEFORMATION OF MATERIALS — $429,000 — 01-2
A. P. L. Turner, U. F. Kocks,
J. L. Routbort, R. B. Schwarz,
G. Gottstein

Investigation of the mechanisms of deformation and mechanical strengthening in metals and ceramics; theoretical and experimental investigations of interactions between dislocations and mobile solute atoms including the phenomenon of dynamic strain aging; analysis of plastic instabilities and texture development in forming operations; experimental investigations of stoichiometry effects on deformation of ceramics; studies of recrystallization and recovery by TEM and HVEM: development of constitutive equations for deformation and creep.

42. METAL PHYSICS — $1,098,000 — 01-3
R. W. Siegel, M. J. Fluss,
N. Q. Lam, J. N. Mundy,
S. J. Rothman, L. C. Smedskjaer,
D. G. Westlake, B. Chakraborty,
T. L. Marcuso, S. Mantl,
T. Schober

The nature and physical properties of atomic defects and their interactions in solids; the atomic mechanisms of diffusion in solids; the nature and properties of metal-hydrogen systems, including the hydrides of intermetallic compounds; investigations of atomic and defect diffusivities, equilibrium defect concentrations, atomic defect interactions with one-another, with solute atoms, and with dislocations, surfaces and interfaces; studies of metals, including bcc refractory metals, alloys, intermetallic compounds, hydrides and glasses, using positron annihilation spectroscopy, tracer diffusion, resistometry, transmission-electron and field-ion microscopy, electron-energy-loss spectroscopy, neutron and x-ray diffraction, backscattering spectroscopy and nuclear reaction depth profiling, molecular dynamics and electronic structure of defects.

43. SUPERCONDUCTIVITY — $250,000 — 01-3
F. Y. Fradin, G. S. Knapp,
K. Kumagai

Studies of the electron-phonon interaction in high Tc, high H_{c2} superconducting compounds; magnetization, nuclear magnetic resonance, and heat capacity studies

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

of local moment interactions in ternary superconducting compounds; extended x-ray absorption fine structure studies of anharmonicity in cubic-Laves phase compounds; phase stability of multi-component, high H_{c2} Chevrel phase superconductors.

44. BASIC CERAMICS — $507,000 — 01-3
N. L. Peterson, W. K. Chen,
K. L. Merkle, D. Wolf,
H. L. Downing, H. Jain,
J. Sasaki

Diffusion mechanisms and point defect studies in metal oxides as a function of oxygen pressure at high temperature using tracer diffusion, conductivity, and ion beam scattering techniques; defect-solute interactions, precipitations of second phases, and defect clustering in oxides; theoretical studies of kinetic processes in off-stoichiometric metal oxides; x-ray scattering studies of low-energy grain boundaries in oxides; TEM studies of dislocation structures of grain boundaries in oxides; theory of grain boundary structures; diffusions of cations and anions along grain boundaries; diffusion mechanisms and impurity interactions in mixed alkali-silicate and -borate glasses; oxidation processes in non-stoichiometric oxides using the environmental cell in the HVEM; preparation of single and bicrystals of metal oxides.

45. ASSISTANCE TO METALLURGY AND CERAMICS BRANCH — $ 94,000 — 01-4
F. V. Nolfi

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

46. NEUTRON IRRADIATION STUDIES — $502,000 — 01-4
T. H. Blewitt, R. C. Birtcher,
M. A. Kirk, Jr., B. A. Loomis

Utilization of the IPNS Radiation Effects Facility for the development of a mechanistic understanding of the effects of neutron irradiation on the physical properties of metals; study of displacement cascades at low temperatures in ordered alloys; studies of neutron sputtering of metals; studies of ordered void arrays in tantalum and niobium in the HVEM; neutron spectrum determinations at a number of neutron sources in the U.S.; neutron damage of semiconductors and superconducting stabilizers.

47. KINETICS STUDIES — $845,000 — 01-4
H. Wiedersich, R. S. Averback,
P. R. Okamoto, L. E. Rehn,
N. J. Zaluzec, W. E. King,
W. Wagner, Z. Wang

Investigations into mechanisms that lead to the formation of defect aggregates, precipitates and other inhomogeneous distributions of atoms in solids without

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

and with displacement-producing irradiation; surface layer modification of alloys by ion implantation and sputtering; solute segregation to internal and external defect sinks; effects of irradiation on ordering alloys and on the microstructure of two-phase alloys; in-situ studies of ion and electron irradiation and ion implantation in the High Voltage Electron Microscope; analytical microscopy; radiation sources include 4 MV Dynamitron-2 MV Van de Graaff dual-ion-beam facility, and 300 keV ion accelerator.

48. HIGH VOLTAGE ELECTRON MICROSCOPE TANDEM FACILITY — $468,000 — 01-4
A. Taylor

Operation and development of 1.2 MeV High Voltage Electron Microscope Facility with in-situ capability for ion implantation, ion damage, and ion beam analysis; the HVEM is currently being utilized for research programs in mechanical properties, radiation damage, oxidation and hydrogenation effects; specimen stages for heating (1000°C), cooling (9°K), straining, gaseous environments and for the ion-beam interface with a 300 kV ion accelerator and a 2 MV tandem accelerator are available for in-situ implantations and irradiations; approximately 50% of the HVEM usage is by non-ANL scientists on research proposals approved by a steering committee for the HVEM that meets every six months.

49. IPNS OPERATIONS — $1,352,000 — 01-4
D. C. L. Price, B. S. Brown

The Intense Pulsed Neutron Source (IPNS) program operates a spallation neutron source for materials science research with neutron scattering and irradiation techniques. Research time on the national facility is prioritized by a national program committee. Available facilities include two liquid helium temperature cryostats and one high temperature environment for fast neutron radiation effects research, a general purpose and a special environment powder diffractometer, a single crystal diffractometer, and a chopper spectrometer.

50. MECHANISMS OF FAILURE OF MATERIALS — $306,000 — 01-5
A. P. L. Turner, J. L. Routbort,
R. O. Scattergood

Investigation of the mechanisms of erosion of ceramics by particle impingement; study of the erosive removal of corrosion product scales from metal substrates and investigation of the effects of radiation on mechanical behavior of metals.

51. CORROSION STUDIES — $472,000 — 01-5
M. B. Brodsky, T. F. Kassner,
K. Natesan, N. L. Peterson,
L. E. Rehn, S. J. Rothman,
H. Jain, P. Marikar, L. Richter

Studies of Ni-Cr alloy oxidation in-situ in the high voltage electron microscope and with LEED, AES, XPS, and analytical electron microscopy; effects of minor

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

and with displacement-producing irradiation; surface layer modification of alloys by ion implantation and sputtering; solute segregation to internal and external defect sinks; effects of irradiation on ordering alloys and on the microstructure of two-phase alloys; in-situ studies of ion and electron irradiation and ion implantation in the High Voltage Electron Microscope; analytical microscopy; radiation sources include 4 MV Dynamitron-2 MV Van de Graaff dual-ion-beam facility, and 300 keV ion accelerator.

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

alloy additions introduced by ion implantation on the oxidation of Ni-alloys using ion beam analysis to study near surfaces segregation; effects of alloying additions on the mechanisms and kinetics of protective scale breakdown for Fe alloys in bi-oxidant environments; grain-boundary diffusion of sulfur in NiO.

Bobby Pundat
-5538

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

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

52. NEUTRON SCATTERING RESEARCH — $2,084,000 — 02-1
T. Brun, P. Dutta, G. Felcher, J. Jorgensen, M. Misawa, C. Pelizzari, V. Rakhecha, F. Rotella and S. Sinha

Neutron inelastic scattering and neutron diffraction are used to study the dynamics and structure of dense fluids and amorphous solids, lattice excitations in crystals, magnetic systems, phase transitions and mechanical properties at high pressures, dynamics of hydrogen in solid and liquid metals, and molecules adsorbed on surfaces. A major effort is devoted to development of instruments to be used with pulsed neutron sources such as IPNS, including a high-resolution powder diffractometer, a crystal analyzer spectrometer, and a chopper spectrometer. Current areas of interest include the structure and lattice dynamics of hydrides, superionic conductors, two dimensional phase transitions in monolayer and sub-monolayer films, ternary superconducting systems, and valence fluctuation materials.

53. MATERIALS PREPARATION AND CHARACTERIZATION — $275,000 — 02-2
S. Susman and D. Hinks

Preparation of metal, insulator and semiconductor single crystals with documented physical and chemical properties; investigations of mechanisms involved in purification and single crystal growth. Materials of current interest are related to studies of fast ion transport in solids, ternary superconductors, and systems which display itinerant magnetism.

54. RADIATION EFFECTS IN INSULATORS — $239,000 — 02-2
W. Primak and E. Monahan

Studies of defects in insulators involving the damage caused by X-rays, γ-rays, neutrons and charged particles, and the relation of such defects to the transport of ions, atoms and electrons. Major areas of activity include radiation induced dimensional changes and stress relaxation of glasses in high radiation level environments; investigations of glasses in connection with their use as waste storage media and diagnostic windows in fusion reactions and relationships of radiation damage to radiation dosages.

55. VERY LOW TEMPERATURE STUDIES $256,000 02-2
P. Roach, L. Jedrzejek
and Y. Takano

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

56. SUPERCONDUCTING AND NOVEL MATERIALS $372,000 02-2
C. M. Falco, K. E. Gray,
R. Kampwirth, M. Khan,
I. K. Schuller and J. Zasadzinski

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

57. CATALYSIS AND SURFACE STUDIES $312,000 02-2
B. Abraham, L. Iton,
K. Miyano, T. I. Morrison
and T. Tokuhiro

Research investigating the physical and chemical processes occurring in two-dimensional systems and interfaces. Research areas include properties of adsorbates on catalyst surfaces such as zeolites, supported metal catalysts and Ziegler-Natta polymerization catalysts; investigations of the rigidity, permeability and ordering of monolayers spread on water; and two-dimensional phase transitions using freely suspended films and monolayers. Experimental techniques include shear measurements of monolayers, resonance methods such as NMR and EPR, and structural techniques such as EXAFS.

58. INTERMETALLIC COMPOUNDS AND HYDRIDES — $456,000 — 02-2
J. Cashion, G. Crabtree, B. Dunlap, W. Johanson, H. Kierstead, D. Niarchos and G. Shenoy

Mössbauer effects and magnetization studies of ternary superconductors such as $ErRh_4B_4$ and related materials; thermodynamic, structural, electronic and magnetic properties of rare-earth (RE) hydrides, and storage hydrides such as RFe_2G_x, RFe_3H_x, RCo_3H_x. EXAFS studies of monomers and dimers of FE isolated in argon and nitrogen matrices; studies of the Fermi surface in metals, alloys and intermetallic compounds via the de Haas van Alphen effect; resistivity and susceptibility at zero and high pressure; measurements of conduction electron effective masses; anisotropy of many-body enhancements; scattering of electrons by impurities, lattice defects and local moments. Materials of interest include Nb, Pt, Pd, actinide materials (U_3As_4, UGe_3, RIr_3); mixed valence and other rare-earth materials (Lu, $LaSn_3$, $CeSn_3$); superconducting A-15 compounds (Nb_3Sb).

59. BASIC STUDIES OF SOLAR MATERIALS — $365,000 — 02-2
M. Grimsditch, L. Guttman, J. McMillan, J. E. Potts and D. Y. Smith

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

60. FAST ION TRANSPORT IN SOLIDS — $255,000 — 02-2
C. Delbecq, S. Susman and L. Boehm

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

61. SOLID STATE THEORY AND COMPUTER SIMULATION — $550,000 — 02-3

L. Guttman, R. Kalia, D. Koelling, M. Parrinello, A. Rahman, D. Y. Smith, and P. Vashishta

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

62. GEOTHERMAL PROSPECTING WITH SQUIDS — $190,000 — 02-5

C. Falco, R. T. Kampwirth, C. W. Lee and I. Schuller

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

ARGONNE NATIONAL LABORATORY

Intense Pulsed Neutron Source Program - 02

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

63. PULSED NEUTRON SOURCE OPERATION $ 870,000 02-1

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

The IPNS Program has the goal of providing an intermediate-flux pulsed spallation neutron source for condensed matter research with neutron scattering and irradiation techniques. Constructed over a 2½-year period at a cost of $8.8M, the IPNS-I facility will be equipped initially with four neutron scattering instruments and capabilities for radiation effects research at high and low temperature. It is run as a national user facility with experiments selected on the basis of scientific merit by a nationally constituted Program Committee. Approximately 40 experiments, mostly involving users from outside Argonne, have been selected for the period October 1981 - March 1982. Relevant Argonne research programs appear under the neutron activities of the Materials Science, Solid State Science and Chemistry Divisions of Argonne National Laboratory.

ARGONNE NATIONAL LABORATORY

Chemistry Division -03-
F. Cafasso - Phone: (FTS) 972-4542 or 312-972-4542

64. CHEMICAL STRUCTURE: NEUTRON AND X-RAY STRUCTURAL STUDIES — $920,000 — 03-1
J. M. Williams, A. J. Schultz, R. G. Teller, M. Beno, P. Vella, T. Morrison, M. Atoji

Research on synthesis and structural characterization of new materials which are either models of catalyst systems or which show catalytic activity or which possess unusual electrical or magnetic properties. Structural characterization of transition metal coordination and cluster complexes; neutron scattering studies of "activated" C-H bonds in hydrocarbon organometallics relevant to Fischer-Tropsch synthesis. Synthesis and characterization of new one-dimensional metal-chain electrical conductors; structure of tetramethyltetraselenafulvalene-based organic para- and superconducting metals. Magnetic properties of rare earth metals and compounds and inorganic bronzes. Design and construction of first neutron time-of-flight, single-crystal diffractometer for studies at the Intense Pulsed Neutron Source.

65. CHEMISTRY OF MATERIALS — $423,000 — 03-2
R. Kumar, P. Cunningham, B. Holt, D. Drapcho, S. Siegel, S. Johnson

Chemistry of atmospheric particulates; formation mechanisms of atmospheric sulfate, nitrates, and organics. Stable oxygen isotope ratio measurements. acidic precipitation chemistry; in situ sampling and real-time characterization of particulates; infrared spectroscopic and chemiluminescent instruments for atmospheric SO_x and NO_x species analysis; phase equilibria in SO_x-NO_x-H_2O-NH_3 systems; heterogeneous and homogeneous conversion chemistries of atmospheric, nitrogen-bearing pollutants; kinetics of gas-solid reactions and role of structural disorder in determining these kinetics.

66. ELECTROCHEMISTRY OF ENERGY STORAGE CONVERSION SYSTEMS & PROCESSES — $586,000 — 03-2
M. Blander, V. Maroni, C. Melendres, Z. Nagy, M.-L. Saboungi, G. Papatheodorou, F. A. Cafasso, J. Settle, R. Yonco

Research on electrode processes and electrolyte chemistry. Electrochemical, spectroscopic (laser-Raman, IR, electronic absorption NMR, ESR, Mossbauer), in situ surface chemical, and theoretical (quantum mechanical, molecular dynamics) investigations. Oxygen reduction electrocatalysis by transition metal organometallics; fast electrode dissolution/deposition reaction kinetics, electrochemical corrosion mechanisms, solvation and associative complexation reaction chemistry in molten salt electrolytes, electrolyte structure, and electrochemical processing.

ARGONNE NATIONAL LABORATORY

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

67. THERMODYNAMICS & CORROSION CHEMISTRY $747,000 03-2
M. Blander, P. A. G. O'Hare,
M.-L. Saboungi, G. Papatheodorou,
L. Curtiss, D. Frurip, E. Veleckis,
W. Calaway, W. Hubbard, R. Yonco

Experimental and theoretical research on the thermodynamic and corrosion properties of a variety of inorganic materials; derivation and testing of statistical mechanical theories of high-temperature multicomponent solutions and vapor molecules; prediction of thermodynamic properties and phase diagrams of sulfide, oxide, and metal systems; experimental tests of theory predictions; quantum mechanical calculations of the structures and stabilities of vapor molecules. Thermodynamics of ionic alloys and binary alloy hydrides; thermochemistry of inorganic sulfides and compounds formed between fission products and glass systems; solution properties of liquid metals and alloys; high-temperature Raman spectroscopy of vapor complexes formed between acidic gases and transition metal and rare earth halides; electronic absorption spectra and thermodynamics of formation of complexes; volatility enhancement by complexes for separation processes; synthesis of metastable alloy compounds by vapor phase condensation; transition metal corrosion mechanisms in liquid metals; role of nonmetals in liquid metals on corrosion; nature of metal-nonmetal interactions in these liquids.

68. HIGH-TEMPERATURE MATERIALS CHEMISTRY $520,000 03-3
K. D. Carlson, D. T. Hodul,
R. J. Thorn, G. E. Murch, E. G. Rauh

Research on solid state chemistry of high-temperature electronic and ionic conducting materials important in energy conversion and storage system. Computer simulation of fast oxygen ion transport; diffusion in highly defective solids. Photoacoustic spectroscopy of semiconducting solids; energy levels, crystal field effects, valence band character of actinide and lanthanide compounds. X-ray photoelectron spectroscopy of opaque powdered ionic compounds; orbital binding energies and ionicities of lanthanide ions. Conductivities of Li-Fe-S phases. Thermodynamic and transport properties of ZrO_2/HfO_2 and ZrO_2/ThO_2 refractories; synthesis of new solids with unusual electrical conductivities and rates of ion transport.

ARGONNE NATIONAL LABORATORY

69. PHYSICAL AND SURFACE CHEMISTRY OF ENERGY SYSTEMS — $680,000 — 03-3

D. M. Gruen, H. E. Flowtow, A. R. Krauss, M. J. Pellin, G. J. Lamich

Charge-transfer processes at surfaces; effects of surface chemistry on excitation, de-excitation, ionization and neutralization mechanisms of sputtered species; charge-transfer from alkali metal monolayers to substrates; mechanisms of surface segregation in alloy systems; mechanisms influencing secondary ion and photon emission; velocity distributions of sputtered atoms via laser fluorescence spectroscopy. Electronic structure of small naked transition metal clusters; cryochemistry of metal dimers in noble gas matrices. Structural and thermodynamic properties of intermetallic hydrides, particularly of Laves and η-phases.

BROOKHAVEN NATIONAL LABORATORY
Upton, Long Island, New York 11973

Corrosion Science Group -01-
J. R. Weeks - Phone: (FTS) 666-2617 or 516-282-2617
M. Suenaga - Phone: (FTS) 666-3518 or 516-282-3518

70. INTERGRANULAR STRESS CORROSION — $300,000 — 01-2
H. S. Isaacs, K. Sieradzki, L. C. Newman

Mechanistic aspects of intergranular corrosion cracking of iron and nickel base alloys in ambient and high temperature water. Studies of effects of heat treatment, stress, surface treatment and sulfur compounds in solution. Electrochemical techniques include ac impedance, polarization measurements and in situ surface scanning for determining location of heterogeneities and location and rates of corrosion. Mechanisms of electrochemical dissolution in simulated cracks and environments and associate salt layer formation. Mechanical tests include crack growth rate measurements constant elongation rates on cracking susceptibility and effects of surface damage as rupture on repassivation. Surface analysis including determination of chromium depletion and grain boundary segregation using scanning transmission microscopy, and x-ray photoelectron spectroscopy.

Materials Science Division -01-
M. Suenaga - Phone: (FTS) 666-3518 or 516-282-3518

71. BASIC PROCESSES AND MICROSTRUCTURAL PROPERTIES OF AMORPHOUS SEMICONDUCTORS — $220,000 — 01-1
R. W. Griffith, R. R. Corderman, M. D. Hirsch, F. J. Kampas, P. E. Vanier

Investigations of the growth, structure, and properties of plasma-deposited thin-film amorphous semiconductors. Studies by optical and mass spectroscopy of processes in the plasma and their relation to film growth and defect formation. Studies of film structure and morphology by electron and optical microscopy, positron annihilation, etc., and of chemical bonding by infrared absorption and electron spin resonance. Measurement of photoelectronic properties and their correlation with structural and bonding characteristics.

72. RELATIONSHIP BETWEEN PROPERTIES AND STRUCTURES — $250,000 — 01-3
D. O. Welch, M. Suenaga, S. Okuda

Fundamental properties of high critical-temperature and critical-field superconductors; effects of strain, disorder, and lattice defects on superconducting properties; theoretical models of interatomic forces, lattice defects, and diffusion kinetics in A15 compounds; annealing kinetics in A15 compounds; studies by electron microscopy of lattice defects in superconducting compounds; properties of composite superconductors; new methods of fabricating superconducting materials.

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

73. PHYSICAL METALLURGY OF METAL HYDRIDE SYSTEMS — $425,000 — 01-3
M. A. Pick, J. R. Bethin, S. M. Heald, D. O. Welch

Studies of physical and metallurgical factors which influence the hydriding behavior of metals and alloys; studies of the role of microstructure, lattice defects, alloying effects, and surface properties on the thermodynamics, kinetics, and mechanisms of hydrogen uptake and release in transition metals, solid solutions, and intermetallic compounds; effect of dissolved hydrogen upon fracture strength; structural and microstructural studies of metal-hydrogen systems using optical, neutron and x-ray diffraction, EXAFS, electron microscopic, and surface sensitive techniques.

74. MATERIALS FOR ELECTROCHEMICAL ENERGY CONVERSION AND STORAGE — $100,000 — 01-3
W. E. O'Grady

The role played by the structure, chemical composition and oxidation states of the surface in electrode reactions is being studied. Electrochemical techniques combined with low energy electron diffraction, Auger electron spectroscopy and x-ray photoelectron spectroscopy are being used. High surface area catalysts prepared by various techniques including ion implantation are also being investigated in an effort to bridge the gap between studies on well defined single crystals and those on microcatalyst particles.

75. RADIATION DAMAGE — $240,000 — 01-4
C. L. Snead, Jr.

Effects of different types of irradiation on critical properties of type-II superconductors; electron, reactor neutron, 14-MeV neutron, 17-MeV, 800-MeV, and 30-GeV proton irradiations; Nb-Ti, and A15 superconductors; defect and microstructure changes in irradiated materials; enhanced diffusion applied to A15 superconductors by solid-state process; application of positron annihilation to defect studies: irradiation-induced defects, and gases in metals. Mechanical properties of various materials using internal friction and dynamical Young's modulus techniques.

76. EFFECT OF MICROSTRUCTURE AND ENVIRONMENT UPON FRACTURE TOUGHNESS — $150,000 — 01-5
D. Gan

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

BROOKHAVEN NATIONAL LABORATORY
Department of Physics -02-
V. J. Emery - Phone: (FTS) 666-3765

77. NEUTRON SCATTERING - MAGNETIC SYSTEMS — $745,000 — 02-1
S. M. Shapiro, J. D. Axe
C. F. Majkrzak, S. K. Satija,
G. Shirane

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

78. NEUTRON SCATTERING - PHASE TRANSITIONS — $805,000 — 02-1
G. Shirane, J. D. Axe, S. K. Satija,
S. M. Shapiro, R. W. Youngblood

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

79. NEUTRON SCATTERING - ELEMENTARY EXCITATIONS IN SOLIDS — $745,000 — 02-1
J. D. Axe, L. Passell, S. K. Satija,
B. H. Grier, C. F. Majkrzak

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

80. NEUTRON SCATTERING - PARTIALLY ORDERED SYSTEMS — $805,000 — 02-1
L. Passell, C. F. Majkrzak,
S. M. Shapiro, R. W. Youngblood, M. Sato

Neutron scattering studies of short-range order and excitations in overlayer films, intercalated layers, and amorphous solids; dynamics of solid electrolytes; dynamics of thin superfluid ^{4}He films adsorbed on graphite.

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

81. EXPERIMENTAL RESEARCH- SPECTROSCOPY OF SOLIDS — $580,000 — 02-2
B. C. Frazer, Y. Fujii, J. B. Hastings, M. Kaplan, W. C. Thomlinson, G. P. Williams, H. Yoshizawa

Structural, dynamic and electronic properties of condensed matter systems studied by x-ray, neutron and VUV spectroscopies. Ferroelectric and martensitic phase transitions. Order-disorder in hydrogen-bonded systems. Intercalated graphite systems. Photoemission spectroscopy of III-V compounds and transition metals. Equipment and technique development for NSLS experiments.

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

82. EXPERIMENTAL RESEARCH - PROPERTIES OF REAL SOLIDS — $460,000 — 02-2
A. N. Goland, K. G. Lynn, P. W. Levy, C. L. Snead, Jr. (DEE); W. J. Kossler (College of William and Mary); R. N. West (U. of East Anglia, UK); H. H. Jorch, P. J. Schultz, and I. K. MacKenzie (U. of Guelph, Canada); D. O. Welch (DEE); M. S. Spergel (CUNY); D. Fischer, L. Granatelli (SUNY-Stony Brook)

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

83. EXPERIMENTAL RESEARCH - ADVANCED MATERIALS SYNTHESIS AND CHARACTERIZATION — $200,000 — 02-2
A. N. Goland, D. E. Cox, A. Moodenbaugh

Synthesis, characterizationn and electrical properties of inorganic materials; fundamental phase equilibria and structural studies by x-ray and neutron diffraction; high-temperature oxide preparation and characterization; application of profile refinement methods to complex oxide structures; studies of structure and disorder in high T_c superconductors; energy-dispersive x-ray diffractometry and planning for beam line at NSLS, monochromator preparation facility for NSLS.

84. EXPERIMENTAL RESEARCH - ALTERATION AND ANALYSIS OF SOLIDS BY ION BEAMS — $180,000 — 02-2
A. N. Goland; H. Herman, S. Prasad, C. R. Clayton, Y. F. Wang (SUNY-Stony Brook); M. Pick (DEE), A. Hanson, K. W. Jones; J. A. Golovchenko (Bell Labs)

Ion implantation and defect profiling in metals and alloys; energy loss of similarly charged heavy ions; alteration of electrochemical properties by ion implantation; XPS and TEM analysis; formation of alloys and precipiates by ion implantation; hydrogen profiling by nuclear reaction techniques; surface phenomena and thin films.

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

85. THEORETICAL RESEARCH $590,000 02-3
V. J. Emery, R. Bruinsma
J. Davenport, G. J. Dienes, H. Hamber
G. Reiter, R. E. Watson

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

86. PARTICLE-SOLID INTERACTIONS - RADIATION EFFECTS RESEARCH $590,000 02-4
A. N. Goland, P. W. Levy, J. M. Loman,
D. R. Dougherty, K. G. Lynn; P. J. Schultz,
I. K. MacKenzie (U. of Guelph, Canada);
R. N. West (U. East Anglia, UK);
C. L. Snead, Jr. (DEE)

Investigations of radiation effects in metals, alloys and semiconductors as a function of incident neutron energy spectrum by positron-annihilation measurements, in situ studies of electron-bombarded natural and synthetic NaCl by measurements of optical absorption and radioluminescence; thermoluminescence of gamma-irradiated quartz and other minerals; dislocation generation in gamma-irradiated crystals; calculation of radiation damage parameters for nonmetals in diverse neutron sources; planning of beam line for studies of transient photon-induced defects in solids and liquids at National Synchrotron Light Source.

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

87. EXPERIMENTAL RESEARCH - SURFACE STUDIES — $545,000 — 02-5
R. H. Cantor, W. Eberhardt, M. El-Batanouny, M. Strongin, S. L. Weng

Use of photoemission to determine the properties of hydrogen and other adsorbates on transition metals; LEED and photoemission studies of structural transitions in overlayers; studies of the mechanism of ion formation during electron stimulated desorption; applications of electron stimulated desorption to studies of bonding geometries; photoemission of adsorbates on metals at cryogenic temperatures; design and construction of VUV beam line for photoemission experiments at NSLS; design and construction of an analyzer for gas phase photoemission.

88. EXPERIMENTAL RESEARCH - SUPERCONDUCTIVITY — $235,000 — 02-5
A. K. Ghosh, Z. Ovadhyau, M. Strongin

Electrical transport properties and localization in disordered conducting systems; the effect of disorder on the superconducting transition, tunneling studies of Coulomb interaction effects in disordered systems; transport and stability in composite superconductors; properties of amorphous silicon.

BROOKHAVEN NATIONAL LABORATORY
National Synchrotron Light Source -02-
A. van Steenbergen - Phone: (FTS) 666-4604

89. EXPERIMENTAL RESEARCH - NATIONAL SYNCHROTRON LIGHT SOURCE, OPERATIONS AND DEVELOPMENT — $2,600,000 — 02-2

A. van Steenbergen, M. Blume, J. Godel, K. Batchelor, L. Blumberg, J. Hastings, M. Howells, H. Hsieh, S. Krinsky, J. Sheehan, W. Thomlinson, G. Williams

Operations of the National Synchrotron Light Source and Research and Development in support of the facility. The operations aspect covers operation and maintenance of the two NSLS electron storage rings and its associated injector combination of linear accelerator - booster synchrotron; operation and maintenance of the photon beam lines of the VUV and X-ray storage rings; and the technical support of experimental users. The development of the NSLS encompasses the further improvement of the storage rings to achieve maximum brightness photon sources and the further development of the photon lines of the facility by means of new developments in high resolution photon optics, state of the art X-ray monochromators, mirror systems, and photon detectors.

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

Don Keefer 8003

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

90. SCALING AND CORROSION IN ENERGY CONVERSION SYSTEMS — $120,000 — 03-1
L. A. Casper, W. F. Downs

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

91. WELDING RESEARCH — $250,000 — 01-5
J. F. Key, H. B. Smartt

Heat source/molten pool interaction studies utilizing high-speed cinematography, optical emission spectroscopy, holography, and infrared thermography to develop process models. Process parameter, material properties, solidification structure relationships. Optical metallographic microstructure characterization; solidification and heat flow modeling. Publication of BES contractor information exchange letter on welding.

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

Corrosion and failure mechanism in environments generic to coal gasification atmospheres. Influences of gas composition with various oxidation and sulfidation propensities. Material variables: Alloy 800H, grain size, carbide concentration and distribution. Test variables: strain, strain rate, stress state, presence of crevices and thermal cycling.

ILLINOIS, UNIVERSITY OF
at Urbana-Champaign
Urbana, Illinois 61801

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

93. LOCALIZED CORROSION OF PASSIVE METALS — $57,000 — 01-1
R. C. Alkire

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

94. CENTER FOR MICROANALYSIS OF MATERIALS — $125,000 — 01-1
H. K. Birnbaum and J. A. Eades

Materials characterization as part of collaborative research with DOE Laboratories and Universities Programs personnel, carried out in the University of Illinois Center for Microanalysis of Materials.

95. RAPID SOLIDIFICATION PROCESSING — $125,000 — 01-1
H. L. Fraser

Development of rapid solidification processing of alloys with powder preparation by laser, spin and centrifugal atomization and subsequent consolidation by dynamic compaction techniques. Characterization of microstructure and measurement of properties developed by heat treatments.

96. SEMICONDUCTOR CRYSTAL GROWTH BY ION BEAM SPUTTERING — $96,000 — 01-1
J. E. Greene

Mechanisms and kinetics of crystal growth. Metastable single crystal alloys for solar and optical applications. Ion beam sputtering, molecular beam epitaxy, laser heating and low energy ion bombardment methods applied to III-V compounds and II-IV-V_2 chalcopyrite systems.

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

Transport processes in undercooled metals and intercalated compounds. Dynamical structure of electrolytes at high temperature and high pressure. Measurement techniques for extreme conditions of temperature and pressure.

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ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (continued)

98. GRAIN GROWTH IN ALUMINA — $47,000 — 01-1
D. S. Phillips

Electron microscopy and diffraction investigation of grain boundaries in sintered ceramics, especially aluminas, both with and without glassy phases.

99. LASER PROCESSING OF MATERIALS SURFACES — $55,000 — 01-1
M. J. Rigsbee and S. H. Risbud

Development of laser processing methods for modification of structure, composition, chemical properties and strength of metallic and ceramic material surfaces.

100. CHARACTERIZATION OF COAL — $50,000 — 01-1
C. A. Wert

Examination of mineral phases in coal, principally sulfides, by analytical electron microscopy. Internal friction peaks observed from the carbonaceous matter are used to investigate features of main-chain motion, appended side radicals, and defect reorientation under stress similar to polymers.

101. HYDROGEN BEHAVIOR IN BCC METALS — $165,000 — 01-2
H. K. Birnbaum

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

102. MECHANICAL PROPERTIES OF MATERIALS — $43,000 — 01-2
J. T. Holder

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

103. COUNCIL ON MATERIALS SCIENCE — $57,000 — 01-2
R. J. Maurer — x 333-7903

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

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (continued)

104. STRUCTURE, CRACKING AND CORROSION OF CERAMIC GRAIN BOUNDARIES — $95,000 — 01-2
S. D. Brown and W. T. Petuskey

Effect of impurities on structure and chemistry of regions contiguous to grain boundaries in SiC and Si_3N_4. Fracture strength toughness, creep and corrosion. Structure of AlN-SiC solid solutions.

105. PHYSICAL PROPERTIES OF CERAMIC MATERIALS — $75,000 — 01-2
W. S. Williams

Strength (flow stress) of carbides, borides, nitrides at high temperatures; transmission electron microscope (TEM and EELS), characterization of defect structures; conductive and chemical properties of carbides; Auger electron spectroscopy and photoelectron spectroscopy for near surface composition and chemical shifts.

106. OXYGEN IN REFRACTORY BCC METALS — $58,000 — 01-3
C. J. Altstetter

Thermodynamics and diffusion of oxygen in refractory metals using solid electrolyte cells. Metal-oxygen and oxygen-oxygen interactions in alloys. Thoria-yttria and zirconia-calcia electrolytes in bulk and vapor deposited form.

107. DEVITRIFICATION BEHAVIOR IN METAL-CONTAINING SILICATE GLASSES — $54,000 — 01-3
H. Chen

EXAFS, small-angle x-ray scattering and SEM investigation of devitrification kinetics and associated microstructural and compositional changes in silicate and borosilicate based glasses containing metal oxides.

108. SOLID DIELECTRICS — $86,000 — 01-3
D. A. Payne

Synthesis, preparation, crystal growth, fabrication, characterization and property measurements on new and improved ceramic materials for energy conversion and detection systems. Relationships between polycrystalline and single crystal properties in electrical ceramics. Flux growth of ferroelectric crystals, hot-forging and extrusion of oriented microstructures in piezoelectric ceramics. Electrocaloric measurements at polar transitions, and field-enforceable anti-ferroelectric-ferroelectric switching.

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (continued)

109. HYDROGEN TRAPPING IN BCC ALLOYS — $53,000 — 01-3
T. J. Rowland

Electronic structure and hydrogen binding energies of trapping sites in binary substitutional solid solutions. Trap characterization by NMR (quadrupole interactions, Knight shift, relaxation time), resistivity vs temperature, EXAFS, and ion probe analysis.

110. MICROWAVE STUDIES OF DISORDERED MATERIALS — $54,000 — 01-3
H. J. Stapleton

Effects of tunneling states and disorder in amorphous semiconductors, fast ionic conductors, and doped crystals using electron spin relaxation, EPR, ENDOR, and microwave dielectric susceptibility in the 0.25 - 25 K temperature range.

111. LOW TEMPERATURE STUDIES OF DEFECT STRUCTURE IN SOLIDS — $101,000 — 02-2
A. C. Anderson

Experimental studies of amorphous or glassy metals, of fast ion conductors, of polymers, composites and ceramics, and of irradiated or deformed ionic and other crystals; influence of defects and disorder on macroscopic properties including specific heat, magnetic susceptibility, thermal and electrical transport, thermal expansion, and ultrasonic and dielectric dispersion at 0.02-200 K.

112. STUDIES OF THE ELECTRONIC STRUCTURE OF METAL SURFACES AND INTERFACES BY PHOTOEMISSION — $22,000 — 02-2
T.-C. Chiang

Synchrotron radiation photoemission investigations of the electronic structures of low-index and stepped/vicinal surface of metals; physisorption and chemisorption kinetics and reactions on these surfaces. EXAFS measurements of surface structures.

113. RESPONSE OF SOLIDS TO ELECTROMAGNETIC RADIATION — $99,000 — 02-2
J. D. Dow

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

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (Continued)

114.	USE OF VERY HIGH PRESSURE TO INVESTIGATE THE STRUCTURE OF MATTER H. G. Drickamer	$146,000	02-2

High pressure studies of the effect of tuning of energy levels and the change of macroscopic variables on atomic and molecular states and processes in condensed phases, applied to: (1) luminescence properties (2) optical effects at a semiconductor-electrolyte interface.

115.	EXCITON COLLECTION FROM ANTENNA SYSTEMS INTO ACCESSIBLE TRAPS L. R. Faulkner	$66,000	02-2

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

116.	IMPURITIES IN SUPERCONDUCTORS D. M. Ginsberg	$60,000	02-2

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

117.	ULTRASONIC INVESTIGATIONS OF THE STRUCTURE OF MATTER A. V. Granato	$153,000	02-2

Investigation by ultrasonic methods of impurity - self interstitial interactions in irradiated metals and semiconductors, and of hydrogen in bcc metals.

118.	DEFECT AND ELECTRONIC PROPERTIES OF SOLIDS D. Lazarus	$108,000	02-2

Atomic mobility in bcc transition metals, metallic glasses, and solid electrolytes. Electrical resistivity and Hall effect in metallic glasses and spin-glass alloys as a function of pressure and temperature.

119.	PROPERTIES OF CRYSTALLINE CONDENSED GASES R. O. Simmons	$122,000	02-2

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

ILLINOIS, UNIVERSITY OF
Materials Research Laboratory (continued)

120.	NUCLEAR MAGNETIC RESONANCE IN SOLIDS C. P. Slichter	$159,000	02-2

Investigations of layered materials with charge density waves, of platinum-alumina reforming hydrocarbon catalysts, and of spin glasses using nuclear magnetic resonance methods.

121.	PHYSICAL PROPERTIES OF ORDERED AND DISORDERED SOLID SOLUTIONS H. Zabel	$74,000	02-2

X-ray and neutron scattering investigations of structural, thermal and vibrational properties of graphite-intercalation compounds.

LAWRENCE BERKELEY LABORATORY
University of California
Berkeley, California 94720

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

122. STRUCTURE AND PROPERTIES OF TRANSFORMATION INTERFACES — 130,000 — 01-1
R. Gronsky

Characterization of the structure and composition of interfaces at high spatial resolution: grain boundaries, interphase boundaries and free surfaces. Determination of the role of interfaces in solid state reactions: structural and compositional evolution accompanying transformations.

123. MICROSTRUCTURE, PROPERTIES, ALLOY DESIGN: INORGANIC MATERIALS — 490,000 — 01-1
G. Thomas

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

124. SOLID STATE PHASE TRANSFORMATION MECHANISMS — 150,000 — 01-1
K. H. Westmacott

Studies of the mechanisms of phase transformations are made using electron optical techniques including the role of crystal lattice defects in precipitation reactions; vacancy-solution interactions in substitutional and interstitial alloy systems; segregation; impurity and minor alloy addition effects. Interrelationships between precipitation sequence, habit plane, orientation relations and crystal structure are being established and compared with theoretical developments.

125. NATIONAL ELECTRON MICROSCOPY CENTER — 505,000 — 01-1
R. Gronsky, G. Thomas and K. H. Westmacott

Organization and operation of a user-oriented resource for transmission electron microscopy. Maintenance, development and application of specialized instrumentation including an Atomic Resolution Microscope (ARM) for ultrahigh resolution imaging, a 1.5 MeV High Voltage Electron Microscope (HVEM) with capabilities for dynamic in-situ observations, analytical electron microscopes for microchemical analysis and support facilities for specimen preparation, imaging analysis, image simulation and instrument development.

ARGONNE NATIONAL LABORATORY

Office of the Director — Kenneth L. Kliewer — Associate Laboratory Director
Physical Research

Lou –

The memo I mentioned to you.

Solar Energy Research Institute
1617 Cole Boulevard
Golden, Colorado 80401
(303) 231-1000

April 19, 1982

Louis C. Ianniello, Director
Division of Materials Sciences
Office of Basic Energy Sciences
U.S. Department of Energy
Washington, D.C. 20545

Dear Lou:

I have read the Panel Report on "Future Trends in Condensed Matter Theory and the Role and Support of Computation" and found it extremely exciting and at the same time very practical.

It is practical in that it points to ways in which we can achieve some of the materials advances which are sorely needed to maintain some of our headway in the materials science field. It is becoming frighteningly expensive to do the experimentation required to develop a new alloy--e.g., to reduce the need for Cr, Co, or Ta in "stainless steels" or to develop a light transmitting material with given optical properties.

The advances of theoretical methods and particularly of theoretical understanding of the nonlinear, non-equilibrium phenomena promise whole new ways of achieving materials goals. The development of powerful minicomputers places the ability to simulate many of these materials concepts in the hands of relatively small groups of researchers.

One could go on at great length on the opportunities presented by present theories and tools. The more practical problem is in the managerial realm, viz., where does one aim among three scenarios; (1) give every theorist who asks for it a CRAY, (2) spread the support uniformly over a myriad of minicomputers, or (3) choose a few major advanced study centers for the large (CRAY-like) programs and carefully select a few other groups to support by funding large minicomputers and staffs of several workers.

My feeling is that the latter approach has greatest promise. The Panel has shown great insight into the opportunities and the needs for this important research area and I would expect them to be valuable guides in

selecting an optimum program of support for this field. A person who might provide great insight into both the science and management of such an effort is George Vineyard who recently returned to research from his post as Director of Brookhaven National Laboratory.

Sincerely,

Gordon

Gordon E. Gross, P.E.
Chief, Materials Research

GEG/mja

Solar Energy Research Institute
1617 Cole Boulevard
Golden, Colorado 80401
(303) 231-1000

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SERI

April 7, 1982

Louis C. Ianniello, Director
Division of Materials Sciences
Office of Basic Energy Sciences
Department of Energy
Washington, D.C. 20545

Dear Lou:

I have, at last, had the opportunity to read thoroughly the report from your committee on Chromium Substitution and Conservation. I have several comments to offer on the report and on research potentials suggested by it. But, first, let me comment that the report is very well written, very stimulating, and seems to have covered the field very well. Your committee deserves congratulations.

The overall topic of material stability in hostile environments has been studied in tremendous detail for many decades. The approach to solutions in such problem areas by using metals has always lead to the difficult compromises between interfacial protection such as the chromium oxide protection in stainless steels and the achievement of suitable bulk properties such as obtained through high alloy steels. As mentioned in the report, the surface protective advantages of silicon and aluminum are completely outweighed by the deleterious effects those two elements have on such bulk properties as weldability and machinability. Clearly, in many of these cases the only solution is through use of a composite in which a surface material of uniquely stable surface properties is attached or cladded onto a bulk material having the desired bulk properties. As soon as such things are done, of course, the problems of diffusion of one set of materials into the other and the subsequent damaging effects arises. When the problems of material durability are attacked by nonmetallic means such as through ceramics, we encounter a new set of problems. Namely, that ceramics are by their nature brittle, that is, they do not have the electron configurations which provide for relatively low energy dislocation movement, hence ductility, such as found in metals. This brittleness on the part of ceramics causes a severe limitation when they are used in structural applications partially because of the fact that designers are accustomed to dealing with forgiving materials such as metal, and have only in the last decade begun to develop the probabilistic design methods which alow use of brittle materials in load bearing structures. This subject of brittle materials in design of structures was studied intensely under Department of Defense programs extending from the early '50's until the late '60's. Many of us who were active in the field at that time recall the "ductile ceramic" dream of the defense establishment. While the works of that period did not achieve the ductility in

ceramics that they originally sought, they did achieve extreme depth of understanding of the mechanical properties and of the physical origins of those properties in nonmetallic materials.

Recent advances in the theoretical aspects of properties of materials and in the laboratory techniques for measuring the microscopic details of mechanical properties and of things effecting them such as diffusion of impurities, diffusion between surface layers, and morphology of surfaces all combine to make the present an ideal time for another frontal attack on the development of new materials and material combinations to achieve desired structural and other properties. Such work could eliminate critical dependence on such unique elements such as chromium. Several Gordon Conferences and Engineering Research Foundation Conferences during the '60's addressed various facets of this subject. It would seem most appropriate to call together another conference where persons, such as those who work on your committee and others who have been deeply involved in the basic physics of materials would be able to discuss the current state of this science and to debate the opportunities for research in this field. They should concentrate on research which could lead to new materials understanding and, eventually, to the solution of problems such as the chromium problem. The meeting should be like the Gordon Conferences in which persons were accepted only by invitation and were chosen on the basis of their ability to probe deeply into the physics and chemistry of material properties. The goal of the meeting would be the development of an integrated research plan which would combine the best of current abilities to tackle the electron theoretical problems of material behavior, the chemical problems of nonmetal activities, the corrosion chemistry problems, and the problems of mechanical and surface testing into a five year research plan. Such a plan, I believe, has extreme promise of delivering the materials solutions sought. If there is any way, Lou, that I could help in identifying some participants for such a meeting or in organizing it, I would be most pleased to do so.

In reading the report, I saw several opportunities for using some of the very advanced surface science techniques that we can supply at SERI on some of the problems, but I think that rather than take individual shots at this large and intriguing opportunity, we would be better off to develop an integrated program in which a selected number of participants would be supported in an integrated program aimed at some very specific things such as the achievement of certain mechanical and other material properties through a long-term research program.

Sincerely,

Gordon

Gordon E. Gross, P.E.
Chief, Materials Research

GEG/mja

Lou
I am keeping a file on this sort of info—
Bob

Japan Times
4/2/82

Ceramic Diesel Engine Developed

NGK Insulators, Ltd. and America's Cummins Engine Co. have jointly developed a highly efficient fuel-saving ceramic diesel engine, the Japanese company said Thursday.

A spokesman for NGK Insulators, a major producer of new ceramics, and the world's top insulator maker, said the new diesel engine, consuming 30 percent less fuel than the conventional diesel engine made of cast iron, has been developed after two and a half years of research and tests under a cooperation arrangement.

The spokesman said NGK Insulators would supply Commins Engines with new ceramics made from zirconia, a material quite low and stable in thermal conductivity, and the U.S. partner would build diesel engines using the new ceramics thus supplied.

He said that in the newly developed engine, the tops of the pistons, the inner wall of the cylinders and cylinder heads have been made using cast iron containing zirconia-type new ceramics.

The spokesman said the two partners are aiming at supplying new ceramics engines to both American and other automakers at an annual rate of one million units from 1985.

famous
Arcade

Japan Times — Feb 2nd 1982

— Material Being Developed as Substitute for Metals —

New Ceramics Creates Stir in Tokyo Stock Market

Reuter-Kyodo

Japanese manufacturers of high performance ceramic products have become a center of attention on the Tokyo Stock Exchange, reflecting the bright prospect of the new basic industrial material as a possible substitute for metals in car engines and other fields.

The Ministry of International Trade and Industry (MITI), which led the government and private collaboration that enabled Japan to become the pioneer in the development of large-scale integration in the 1970s, last year launched a 10-year program involving 15 high-technology companies to develop more advanced ceramics.

"The ultimate aim of the project is to make fine ceramics as strong and applicable as metallic materials," said a spokesman for MITI's Agency for Industrial Science and Technology, which is coordinating the plan.

Two of the participating firms, Kyoto Ceramic and NGK Spark Plug, have already announced development of experimental ceramic engines of 2,800 cc and 50 cc capacity, which helped boost what stock market analysts called the ceramic boom.

Among the other participants are Toyota, Japan's largest car manufacturer, Ishikawajima-Harima Heavy Industries, Toshiba, NGK Insulators, Asahi Glass Co., Kobe Steel, Sumitomo Electric Industries and Shinagawa Refractories.

While conventional or old ceramic products such as china and bathroom tiles are fragile, new ceramics produced by high technology treatment processes have a high resistance to heat and corrosion and sometimes have optical electric or magnetic characteristics, scientists said.

New ceramics, already widely used in integrated circuits and circuit components, are based on alumina while ceramics for new engines are made from silicon nitride, which can be produced by combining silicon and nitrogen.

Silicon nitride ceramics have improved heat resistance and less fragility in rapidly changing temperatures, thus making them useful in engines and spacecraft re-entry vehicles such as the space shuttle Columbia.

The highlight of the competition among Japanese companies is development of silicon nitride ceramics. NGK Spark Plug was the first company to test-run successfully an all-ceramic engine, using the new type of material

Kyoto Ceramic was the first actually to run an experimental car powered by an all-ceramic diesel engine, also made from silicon nitride, a company spokesman said.

The engine consumes 30 percent less fuel than conventional metallic engines because it requires no cooling system.

One stock analyst said investors as well as carmakers know it will take a long time to go into the commercial production of all-ceramic engines. "But people like dreams," he commented.

The revenue from ceramic products of major manufacturers represents only a small percentage of total sales and the Nikko Research Center has described as exceptions Kyoto Ceramic's 85 percent in the last financial year and NGK Spark Plug's 38 percent.

Amid new year projections by leading share analysts that ceramic producers would be favorite issues throughout 1982, the share prices of three companies touched record levels in the first business week of the year.

NGK Insulators rose to 566 compared with 453 at the start of 1981 trading, Shinagawa Refractories went up to 564 from 340 and Toshiba Ceramics, a member of the Toshiba group, stood at 1,050 against 711.

Nikko Research said sales of fine ceramics were forecast to increase to ¥700 billion ($3.14 billion) in 1985 from an estimated ¥180 billion ($807 million) last year and ¥140 billion ($628 million) in 1980.

It said the projected high growth of ceramic production was in line with the continued expansion being experienced in the Japanese electronics industry.

Analysts said ceramic issues on the stock exchange were expected to be unaffected by uncertainties in the Japanese and overseas economies because development of high-performance ceramics would have to be pursued whatever the circumstances.

#1.649 M cut. BES

	NS		MS	CS	EMG			MEP	BEP	Total	
	SB	ER			E	M	G				
Ames		20	50	15						85	4
ANL			90	25						115	7
BNL			60	10						70	-
INEL										0	
LANSL		57	30							87	3
LBL			60	15						75	1
LLL		13	10				60			83	2
Mound			0							0	
ORNL	50		95	10						155	
PNL		40	20							60	5
Sandia A			10							10	0
Sandia L			10	10						20	1
SERI				10						10	1
subtot	50	130	435	95			60	0	0	770	
LLL			20								
Nash	30	50	215	374	8	8	24	70	80	879	
ND											
Total	80	180	670	469	8	8	84	70	80	1649	

Preliminary Program
Working Group Meeting on Low Temperature
Neutron Irradiation, May 17-19, 1982

Monday AM - Introduction
Review of Past Scientific Contributions
Discussion of Future Scientific Directions

PM - Review of Research Overseas
Fusion Materials Program
Current and Potential Facilities

Tuesday AM - Discussion of Research and Facilities, formulation of report outline

PM - Preparation of Draft of Report (individual)

Wednesday AM - Final Draft, Conclusions, Recommendations

Department of Energy
Washington, D.C. 20545

March 5, 1982

Professor R. W. Balluffi
Department of Materials Science
and Engineering
Massachusetts Institute of Technology
Cambridge, Massachusetts 02139

Dear Bob:

I appreciate your willingness to serve as Chairman of the Low Temperature Neutron Irradiation Working Group. I understand from Don Parkin that you have agreed to accept this task and that you both have been working hard on developing a plan for the meeting to be held May 17-19, 1982.

The Council on Materials Science panel report on The Effects of Irradiation on the Structure and Properties of Materials in one conclusion stated that a low temperature neutron irradiation facility is "...an essential resource for the indefinite future..." and gave a brief description of the characteristics that such a facility should have. With the projected near term phase-out of IPNS-I at Argonne National Laboratory, where the only operating low temperature neutron irradiation facility is located, the topic of low temperature neutron irradiation research requires careful examination at this time. I am, therefore, requesting that the Working Group review the past scientific contributions of low temperature neutron irradiation research; assess the importance of future scientific directions both in basic and applied research; identify the current and potential facilities options to meet the agreed upon research needs; and recommend the most reasonable course of action in the area of low temperature neutron irradiation research.

We have taken steps to coordinate this meeting with the fusion materials program since they have a requirement for obtaining neutron irradiation data at low temperature on materials to be used in superconducting magnets.

I am looking forward to attending your meeting. The subject is extremely important and the timing is critical. You and your colleagues should know in advance that we will do our best to carry out the major conclusions of the study. Please let me know if I can be of further assistance.

Sincerely,

Louis Ianniello

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

DOE F 1325.8
(7-79)

U.S. DEPARTMENT OF ENERGY

memorandum

DATE: March 5, 1982

REPLY TO ATTN OF: ER-13

SUBJECT: Delineation Between Research Done in the Materials Sciences Division (BES) and the Materials Program of Fossil Energy

TO: Richard H. Kropschot, ER-10

The Materials Sciences research program is aimed at understanding phenomena, materials or properties of materials in certain environments of interest to the fossil energy program. Most of the program, however, is multitechnology oriented, not readily identified with any energy technology or directed at other energy technologies (fusion, solar, fission, etc.). That part of the program that is considered to underpin the fossil energy program seeks to undercover new knowledge or new applications of existing techniques to build a base of information on which new solutions to fossil energy materials problems or new opportunities are possible. It is generic research primarily. Conditions are chosen with the ultimate aim of being able to extrapolate to more general conditions.

On the other hand, there is a need in the materials field to be more specific with regard to actual operating conditions, to test materials which are commercial alloys or to develop practical materials. Much of this research is considered long term development or applied research. Industry considers this too long term and too risky. The fossil energy program should and does support this type of research and presently does not support research primarily aimed at understanding phenomena, i.e., basic research. Only a small fraction of the needed long term development or applied research is currently being funded by the fossil energy program. There is no significant overlap between the two programs. This conclusion is based on information obtained from discussions with contractors, headquarters staff personnel, attendance at technology review meetings and numerous contacts between Materials Sciences staff personnel and fossil energy staff personnel via EMaCC meetings, contractor meetings, research assistance task force meetings, etc.

Examples of Programmatic Interactions

- Erosion:

  FE - Evaluates candidate materials for valves and nozzles at Battelle-Columbus, the U.S. Bureau of Mines and LBL.

  BES - Investigates mechanisms of erosion at ANL, ORNL, LBL, and universities.

  BES started the program at LBL first and now FE is the major supporter of the group at LBL because of its applied character now. On the other hand, a program at Notre Dame University on abrasive wear was terminated in FY 1981 and BES initiated a contract to continue the basic studies.

- Corrosion:

  FE - High temperature gaseous corrosion of heat exchanger materials; slagging corrosion of refractories for pressure vessel linings; stress cracking of fractionation column materials; failure analysis of coal liquefaction components; and hydrogen attack (ANL, ORNL, Cornell, U of California/SB), all with emphasis on engineering and materials development.

  BES - Studies are underway in about 20 separate projects at universities and laboratories to understand mechanisms of grain boundary penetration, sulfidation, hydrogen attack, hot corrosion, corrosion-related diffusion phenomena, etc.

  At ANL the FE program on materials behavior in coal-gaseous conversion environments is conducted by the same scientists investigating the mechanism of oxide film breakdown on corrosion resistant alloys in multicomponent gas environments for the BES program. At Sandia-L, the BES program on in-situ characterization of combustion surfaces (using laser Raman scattering) is coordinated with FE work at the Combustion Research Facility and FE supported coatings development.

- Other areas of close interaction include mechanical properties of pressure vessel materials, catalysts, physical structure of oil shale and coal, welding and ceramics including materials for MHD. In the area of physical structure of oil shale/coal, the type of research done in Materials Sciences and not in FE includes internal friction studies and neutron/x-ray scattering to study pore/maceral distributions.

Research Needs

Past history with fossil (and nuclear) industries shows that plant down time is associated with conventional equipment/components being operated under non-conventional conditions. The costly effects of this down time do not have to be repeated here. The overwhelming conclusion by all the studies and reviews I have seen is that materials performance and reliability is a major problem in the advanced fossil energy conversion and utilization systems. Although basic research can and does contribute to solving this problem, it is primarily a materials development, applied materials requirement. There is a need to develop new higher performance materials and determine materials performance and reliability under realistic conditions. All of this is relatively long term and will not be done by industry with their funds. The Fossil Energy program is supporting some of the research needed, but needs to do much more. Insufficient funds have been allocated to applied fossil energy materials research. Some additional information and references are given in the attached memorandum to me from Dr. Stanley Wolf.

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

Attachment

DOE F 1325.8
(7-79)

U.S. DEPARTMENT OF ENERGY

memorandum

DATE: March 5, 1982

REPLY TO ATTN OF: ER-131

SUBJECT: Comparison of Materials Programs in DOE-Basic Energy Sciences and Fossil Energy

TO: Louis C. Ianniello, ER-13

Introduction

This objective/goal for materials research and development supported by DOE-BES and DOE-Fossil Energy (FE) are stated in the first paragraph below. Further delineation of these programs is given through specific examples in the following section. Finally, some FE-related basic research areas considered worthwhile for receiving increased support are identified.

Objectives/Goals

The BES Division of Materials Sciences supports fundamental research in energy-related materials problem areas and exploits the unique capabilities and facilities in DOE laboratories for this research. The goal is to provide a foundation for the technology base needed for energy technologies. Emphasis is placed on long range interdisciplinary research contributing to several energy technologies, though some work addresses specific technologies. For the DOE-FE Materials Program[1], "...the objective...is to conduct...research and development (R&D) on materials for fossil energy applications focussing on the longer range needs of the various fuel technologies. The program will include research aimed toward better understanding of material behavior in fossil energy environments and the development of new materials capable of substantial enhancement of plant operations and reliability". Overlap but not duplication of the BES and FE programs exists to a small measure; continued coordination[2] between these has led to a demarcation of applied efforts being supported in the main by FE and basic research by BES.

Delineation between the two programs

This is reflected in specific examples given below. The areas have been selected from published reports[3,4] citing technology needs important for coal conversion.

1. Erosion[3] (of materials handling equipment, valves, and pressure vessel internals): FE-contractors evaluate candidate component materials (e.g., valve and nozzle materials at Battelle Columbus[5] and Bureau of Mines[5]) whereas BES contractors examine mechanisms of erosion[6] and wear in ductile and brittle materials (e.g., ANL, ORNL, Carnegie Mellon University). Recent changes in two projects clarify further the basic vs applied thrusts of the BES and FE programs. A project at Notre Dame on "Microstructural Effects in Abrasive Wear" contained both applied and basic aspects[5]; the FE contract for this terminated in 1981 and a BES contract to continue a basic study[6] was initiated. Conversely, a project at Lawrence Berkeley Laboratory on "Erosion-Corrosion-Wear"[6] was tending towards applied rather than basic research; this project is being phased out of the BES program in FY 83 and the more applied tasks will continue under an existing FE contract with the same principal investigator.

2. Corrosion[3]: The FE program[5] emphasizes engineering and development (e.g. high temperature gaseous corrosion of heat exchanger materials and slagging corrosion of refractories for pressure vessel linings [ANL] and stress cracking of fractionation column materials and failure analysis of coal liquefaction components [ORNL]). It also includes research (e.g., on hydrogen attack at universities - Cornell, California-Santa Barbara). The BES program[6] includes ~20 research projects addressing, mechanisms of corrosion (e.g., grain boundary attack, oxide scale development and breakdown, associated diffusion phenomena).

3. Structural stability[3] and reliability (of pressure vessels, internals, and heat exchangers): The FE effort[5] aims at actual or simulated component evaluation (e.g., NDE detection of wear in piping [ANL], creep-rupture of refractories (Ames Lab) and of heat exchanger tubing in a simulated gasifier environment (INEL), and fracture toughness of commercial or slightly modified pressure vessel steels [Westinghouse]). The BES materials thrust in NDE[6] is focussed on quantifying the interaction of the probe signal with defects in materials so that the defect and residual materials properties can be characterized. The large BES program on mechanical properties is dominantly generic research, i.e., effect of grain boundary impurities or stress state on cavitation and cracking, environmental influence on enhancing deformation vs fracture.

4. Instrumentation: FE has an instrumentation program which has identified[4] needed improvements, including sensor materials, and which has acknowledged[4] that "...most of the materials and instrumentation development work is short range in nature...". The BES program has maintained long term support for materials and techniques which are pertinent to this area. For example, small angle neutron and X-ray scattering have been coupled to determine pore size and oil distribution in oil shale (ORNL); semiconductor characteristics have been tailored by ion, laser, and electron beam processes (ORNL, San-A).

5. Other Areas: Fabrication technology and ceramics have also been identified[3] as key needs for coal conversion technology. A comparison of BES vs FE support in this area reveals the same basic vs applied demarcation shown in items 1-3 above. BES has also initiated materials research activities in other areas related to FE, i.e., catalysts and coal structure, involving as an integral manner several fundamental research methods for surface and bulk analysis (electron microscopes, research reactors, and laser diagnostics).

Basic Research Needs

In order to support the range of basic and applied work needed the BES Division of Materials Sciences should continue its emphasis on basic research and FE its focus on the more applied aspects of longer range technology needs. However, should DOE-FE wish to emphasize basic research, it certainly should learn more about our program and seek out areas which we are not addressing adequately. Some of the more important are: corrosion in coal liquefaction fluids, erosion in three phase (liquid, solid, gas) streams, erosion, ceramic composites, sulfur probes, processing heavy section steels for improved fracture toughness, NDE, among others.

Stanley M. Wolf
Division of Materials Sciences
Office of Basic Energy Sciences

References

1. R. A. Bradley and R. R. Judkins, "Program Plan for the AR&TD Fossil Energy Materials Program", ORNL/TM 7206 (July 1980); quotation from pages 1-2.

2. Coordination between FE and BES materials programs through the following:

   a. Energy Materials Coordinating Committee.
   b. BES attendance at FE program reviews, e.g., annual conferences on Materials for Coal Conversion and Utilization.
   c. BES-FE joint contractor meetings, e.g., one on weldments in pressure vessels planned for August 1982.

3. R. T. King and R. R. Judkins, "Fossil Energy Materials Needs Assessment", ORNL/TM-7273 (July 1980).

4. Materials for Instrumentation for Fossil Energy Technologies, National Bureau of Standards, NBSIR 81-2348 (August 1981); quotation from page 4.

5. Proceedings, Sixth Annual Conference on Materials for Coal Conversion and Utilization (October 1981), no report number.

6. Materials Sciences Programs FY 1981, U.S. Department of Energy, DOE/ER-0106 (September 1981).

The many accomplishments flowing from research carried out by this program during the last year include:

o Development of a new method for fabricating a class of materials called intermetallic compounds. These compounds have excellent corrosion resistance which is important for energy applications but have seen limited use in the past because of their brittleness.

o Discovery of a new class of chemical extractants that can be used to recover and purify selected valuable elements, such as palladium from nuclear waste solutions.

o Development of a liquid membrane for enrichment of the oxygen content in air. Oxygen is important for efficient combustion, and crucial for high Btu coal gasification. The new liquid membrane is an improvement over state-of-the-art solid membranes, with it, oxygen-enriched air could be produced at great savings in energy and cost compared to present day technology.

o A micro-organism has been discovered that is capable of converting the waste gas, carbon monoxide, into commercially-valuable larger molecular weight chemicals such as acetic acid. This conversion, which can be accomplished without energy input from other sources, has implications for the chemcials and plastics industries among others.

o A combustion process diagnostic technique that, by improving our understanding of flame constituents and characteristics, ~~is expected to~~ will help build our ~~result in an~~ ability to tailor fuels to specific needs and reduce pollutant emissions.

MAR 4 1982

DOE F 1325.8
(7-79)

U.S. DEPARTMENT OF ENERGY

memorandum

DATE: March 3, 1982

REPLY TO ATTN OF: MA-82.1

SUBJECT: FY 1982 General Reductions

TO: Assistant Secretary for Management and Administration
Assistant Secretary for Nuclear Energy
Assistant Secretary for Environmental Protection, Safety and Emergency Preparedness
Assistant Secretary for Conservation and Renewable Energy
Director of Energy Research

On Saturday, February 27, 1982, Messrs. Tribble, Edmondson, and I met with Mr. Fazio, Congressman from California, and staff members of the House Subcommittee for Energy and Water Development Appropriations and Science and Technology to discuss the Department's proposed allocation of the FY 1982 general reduction. The staff indicated that DOE's application of the $49 million general reduction to the Energy Supply Research and Development Operating Expenses Appropriation was too heavily weighed against Solar and Renewable Programs. They described the problems with support of the FY 1982 bill and the potential problems with the bill for FY 1983 if the reductions to Solar were allowed to stand.

The staff and I have agreed to an alternative method of applying the reduction which has the effect of increasing the funding for Solar and Renewable Programs and reducing the funds for the other programs in that account. The attached table reflects that method. Essentially, unobligated balances are applied first and the remaining reduction is based on a percentage of the FY 1982 appropriation amounts for each program area.

The programmatic changes required by this new allocation are to be submitted to the Budget Officer by March 9, 1982, and reflected in your normal March input for the April Approved Funding Program (AFP). Your staff will be contacted by the appropriate Controller representatives to coordinate these changes. You are reminded that AFP changes resulting in a decreased allotment must be specifically cleared with the allottee.

This change also impacts the potential solution to the funding problem we have in Departmental Administration. With your help, we had set aside more than $4 million from unobligated balances as a partial solution to the total $15 million problem. Due to the current revision to the allocation of the FY 1982 general reduction, those amounts will be returned to you to offset some of the impact. You should be aware, however, that it may be necessary in the near future to assess each program an appropriate share of the $15 million problem.

Any questions on this matter should be addressed to the Budget Officer.

Guy W. Fiske
Under Secretary

Attachment

FY 1982
ENERGY SUPPLY OPERATING EXPENSES
SUMMARY

($ in Thousands)

	1982 Appropriation $	(%)	Unobligated Balances	1981 Deferral General Reduction	Unobligated Balances Available	Additional Reduction	Revised 1982 Deferral Reduction	FY 1982 Net Available	Original 1982 Deferral Reduction	Change in 1982 Deferral Reduction
Renewables	$ 381,086	(17.9)	$ 95,150	$ 83,162	$ 11,988	$ 2,588	$ 14,576	$ 378,498	$ 29,537	$ -14,961
Nuclear	989,610	(46.6)	31,630	15,026	16,604	6,737	23,341	982,873	17,337	+6,004
Energy Research	255,511	(12.0)	7,027	5,000	2,027	1,735	3,762	253,776	---	+3,762
Magnetic Fusion	292,700	(13.8)	3,078	2,500	578	1,995	2,573	290,705	---	+2,573
Environment	207,100	(9.7)	3,739	-0-	3,739	1,402	5,141	205,698	2,519	+2,622
Environmental Protection, Safety and Emergency Preparedness	53,891		2,111	-0-	2,111	365	2,476	53,526	543	+1,933
Energy Research	153,209		1,628	-0-	1,628	1,037	2,665	152,172	1,976	+689
TOTAL	$2,126,007	(100.0)	$140,624	$ 105,688	$ 34,936	$ 14,457	$ 49,393	$2,111,550	$ 49,393	-0-
General Reductions:										
FY 1981 Deferrals	$ -105,688									
FY 1982 Deferrals	-49,393									
	$1,970,926									

501,419 BES
(400,596) Proj Dev
989,167 ERA

BO BH reduction

15 mil 47

1.649 reduction BES

$\frac{240}{4} = 60$

due ~~[illegible]~~ by 8th

Reprogram for Dept. administration for FY-1982 — 250,000 from director's reserve (470 K)

All shortfall of $15 M

- 6.5 M from ER – pending
- 4.175 from F Supp
- 2.460 from GS
- remain from NE
- 15.00

prorate exclude weapons, SPO, enrichment

AT – appeal? to Fish: Del [illegible] outcome

Take all out of OPF – tentative

→ may tax BES about 2 – equipment. 6.5 unobligated as Jan 31

due by 9th AM

NS	4.2
MS	9.8
CS	50
FMG	.7
AFP	—
BEP	.2

.5

	ANL	BNL	ORNL	
NS	.6	.9	2.7	
MS	3.6	2.8	3.5	
CS	1.5	2.1	1.4	
FMG	.4	.1	.2	1.65
	6.3	5.9	7.8	= 20.
	33.3	33.8	41.2	8 1/2%
	19.%	17.5%	18.9%	
	.519	.487	.645	= 1.649
	5.72	5.41	7.15	
	17.2%	16.1%	17.3%	

When do we alert [illegible] NS15, [illegible], 2 reaction

[illegible] down [illegible]

KC-01

ANL	602,280
BNL	873,485
ORNL	2,727,562
subtotal	4,203,327
TOTAL	7,609,485

KC-02

ANL	3,567,609
BNL	2,768,810
ORNL	3,471,259
subtotal	9,807,678
TOTAL	18,674,829

KC-03

ANL	1,504,851
BNL	2,093,807
ORNL	1,378,040
Subtotal	4,976,698
TOTAL	12,324,300

KC-04

ANL	361874
BNL	97,204
ORNL	237,237
Subtotal	696,315
TOTAL	6,739,075

KC-05

BNL	5,638
TOTAL	4,150,670

KC-06

BNL	223399

U.S. Department of Energy
ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue, Argonne, Illinois 60439
Telephone 312/972-

February 3, 1982

TO: K. L. Kliewer

FROM: G. H. Lander

SUBJECT: Foreign Travel

Following our discussion I have put down some thoughts towards justifying my proposed visit to ILL.

(1) Science

One central question concerning actinide system is related to the form of the dynamical response function. Efforts to understand this focus on two things: (a) the form and temperature dependence of sharp spin waves. These measurements are best done with a single crystal and a 3-axis spectrometer at a reactor. We have such an experiment scheduled for IN8, the most intense 3-axis at the ILL. The crystal was grown in Zurich. Efforts to grow such crystals at ANL have not been successful and have now been abandoned. [See my note about reduction in sample effort in scattering group in MSD.] Furthermore, the experiment requires application of 10T and such fields do not exist at a U.S. neutron facility. (b) the form and temperature dependence of the diffuse response. The measurements are best suited to a pulsed source and one latest publication describes work with M. Loewenhaupt, who is coming from Julich for a year into MSD, on a time-of-flight spectrometer IN4 at ILL. Two proposals on this work have been submitted to IPNS, and Sinha, Price and myself plan to run UO_2 and $UA\ell_2$ in instrument time on the LRMECS in late February. A similar experiment by S. Shapiro of BNL on Ce-Th alloys is scheduled for later.

The second experiment on the chevrel phase materials is also of great interest to ANL programs in both MSD and SSS. We are here using extremely advanced technology but there is no reason that IPNS should not be able to do these experiments just as well once we have built up the necessary ancillary equipment on the SAD.

The "linkage" between scientific effort at IPNS and other places is of crucial importance. I have already covered the response function and chevrel phase work. Our work on α-U is another example. First at CP-5, then at ORNL (mentioned in Brinkman report with no acknowledgment of ANL role), then at ILL, where a really new discovery was made, back to ORNL and now a proposal on the SCD at IPNS. Yet another example is the anharmonic effects in AB_3 systems. First realization of possibility from CP-5 work, then proper experiments at ILL, follow up with Stassis and Loong at ORNL on $CeSn_3$ and $LaSn_3$; interest of

Jerry Cohen, and now proposal to IPNS with Cohen and his student on martensitic transformation in $PtFe_3$. We are hoping the student will spend the summer here. I believe Loong's enthusiasm to come here stems largely from his interaction with Faber and myself, on a program that got underway using epithermal (0.5 Å) neutrons at the ILL hot source.

I apologize for these sounding like plots from a John le Carre novel. They should rather be looked on as the wares of a used-neutron salesman.

(2) ANL-ILL Interface

The ILL represents the most advanced thinking in the world today on neutrons. Neutron guides, supermirrors, spin-echo devices, and multi-detectors represent just some of the novel efforts underway. The permanent staff is ~ 400 with 80 Ph. D's, all in aspects of scattering (or nuclear physics). We stand to benefit greatly by keeping informed of this technology, and also that being developed at the Rutherford/Harwell complex. For example, in two areas, the search for the electric-dipole moment on the neutron and the search for nuclear magnetic ordering in ^3He, we are in direct competition with Grenoble. They have more manpower and money in both and a big headstart. If either of our efforts request substantial resources from the general IPNS effort how do we deal with it? My judgement on such requests, which I anticipate, will be based partly on what I know about these other efforts. How much do you spend to come second?

(3) Personnel Recruitment

With IPNS budget profile so serious we cannot hire permanent staff, so must strive to have visitors. While in no way neglecting U.S. candidates the extreme shortage makes it almost impossible to fill our needs. Two will be interviewing for the postdoc position in February. At the present time we have approached the following people in Europe:

C. Windsor (AERE), M. Loewenhaupt*(Julich), Blankenhagen* (Karlsruhe), S. Howells* (Rutherford), S. Burke (ILL), J. Pannettier (ILL), J. Zaccai (ILL), D. Worcester (ILL), A. Hewat (ILL).
Not all will come, of course, but they would greatly aid our program. J. Copley from McMaster, previously ANL and ILL, is signed up for 2 months from June.

In this regard you should know that LANL have a collaborative agreement with Rutherford (that's where they got Andy Taylor, one of their best) and have given consultantships to R. Pynn and F. Mezei of ILL. Both the latter are friends of mine, Roger is a collaborator on the chevrel phase experiments, and they will visit ANL on the way to or back from LANL, and hopefully run experiments here. It is not my intention to grant open lucrative consultantships because we have an excellent in-house staff. LANL doesn't, but seems to have the money to get people there.

You should realize that IPNS has a credibility problem after the Brinkman report. Harold Wroe of the Rutherford, for example, called me up to ask if we were not closing down this October. It is of great importance that we continue to keep a highly visible profile by bringing neutron people here from the U.S. and abroad and showing them how things are going and what our

* Definite

plans are. LANL personnel have continued to go to conferences and display future grandiose plans, leaving the impression that ANL is busy doing a few things on a small unreliable accelerator before closing up the shop.

GHL:jcg

cc: File 2.13.3

P.S. The above written before DOE visit but still valid. Incidentally, Mezei has submitted a proposal to do an experiment at IPNS before going to pick up his check at LANL.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division

126. IN-SITU INVESTIGATIONS OF GAS-SOLID REACTIONS BY ELECTRON MICROSCOPY — 60,000 — 01-1
J. W. Evans and K. H. Westmacott

The investigation of in-situ reactions using an environmental cell in the 650 kV and new 1.5 MeV high voltage electron microscopes. Emphasis is on the investigation of the effect of microstructure, e.g., dislocations, grain boundaries, and surfaces on reactions between gases and solids. Initially, nickel oxide reduction by hydrogen has been studied in both ex-situ and in-situ experiments. Subsequently oxidation, sulfidation, and other reactions significance to materials performance in energy conversion systems will be investigated.

127. LOCAL ATOMIC CONFIGURATIONS IN SOLID SOLUTIONS — 30,000 — 01-1
D. de Fontaine

A computer simulation of a two-dimensional two-component crystalline solid solution has been performed. Statistics of local order were determined by use of the cluster variation method in the square-cluster approximation. Pair interaction parameters to ninth neighbor have been obtained. Thus, the method shows promise for simulation of electron optical and X-ray diffraction contrast from real crystals. Cluster variation methods are also being used to calculate the influence of atomic ordering on the ferromagnetic transition in an fcc crystal containing two magnetic components.

128. THEORETICAL PROBLEMS IN ALLOY DESIGN — 440,000 — 01-2
J. W. Morris, Jr.

Physical metallurgy: study of phase transformations, microstructures, and mechanical properties of materials using modern experimental and theoretical methods. Alloy design: development of new engineering alloys and welding processes for advanced energy systems.

129. STRUCTURE-PROPERTY RELATIONSHIPS IN SEMICONDUCTOR MATERIALS — 255,000 — 01-2
J. Washburn

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

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division

130. MECHANICAL PROPERTIES OF CERAMICS — 195,000 — 01-2
A. G. Evans

Study of brittle fracture mechanisms and of creep and creep rupture processes in ceramic polycrystals at elevated temperatures. Studies of pore and grain evolution during final stage sintering. Development of a scientific basis for relating processing to mechanical failure at high temperatures.

131. ENVIRONMENTALLY AFFECTED CRACK GROWTH IN ENGINEERING MATERIALS — 30,000 — 01-2
R. O. Ritchie

The program involves an investigation into mechanical, metallurgical and chemical factors governing mechanisms of monotonic and cyclic environmentally affected crack growth in both gaseous and aqueous atmospheres for a variety of steels ranging from lower-strength pressure vessel steels to ultrahigh-strength aerospace materials. Principal emphasis is on defining the role of environment and microstructure on microscopic crack closure mechanisms and their effect on subsequent crack growth behavior, specific to the ultralow growth rate, near-threshold regime in fatigue (below 10^{-5} mm/cycle) for inert, moist and hydrogen gas environments. Characterization of growth rate behavior will be achieved through the use of linear elastic and elastic-plastic fracture mechanics, microstructural and surface chemistry analysis, and detailed fractography. Based on the mechanistic understanding obtained, guidelines will be sought for the development both of improved failure prediction and improved alloy design of environmentally sensitive materials.

132. INTERFACES AND CERAMIC MICROSTRUCTURES — 45,000 — 01-3
J. A. Pask

Kinetics and mechanisms of solid state reactions, nucleation and growth phenomena, and distribution of phases in multiphase ceramic systems whose principal phase constituents are within the Al_2O_3-SiO_2 system. Thermodynamic considerations of sintering with a liquid phase. Mechanisms of corrosion of ceramic materials. Thermodynamics and kinetics of electrochemical reactions at glass-metal interfaces.

133. HIGH TEMPERATURE REACTIONS — 250,000 — 01-3
A. W. Searcy

Recent studies have focused on the thermodynamics and kinetics of decomposition reactions. Emphasis is placed on coupling kinetic studies with measurements of properties of the solid product of decomposition reactions as functions of the temperature, reactant particle size, particle bed size, and product gas pressure. Also under study are surface kinetics, solid solution thermodynamics, the catalysis of metal sulfate decomposition, the catalysis of gas reactions by solid surfaces, and vapor transport through porous solids.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division

134. CHEMICAL PROPERTIES OF CERAMIC ALLOYS AND PROCESSING OF CERAMIC MATERIALS — 100,000 — 01-3
L. C. De Jonghe

Mechanisms and kinetics of gas-solid reactions, in particular reactions between oxides and hydrogen or CO/CO_2; study of these reactions by means of thermogravimetrical analyses and microscope techniques, including high-resolution transmission electron microscopy and analytical scanning transmission electron microscopy.

135. STRUCTURE AND ELECTRICAL PROPERTIES OF COMPOSITE MATERIALS — 105,000 — 01-3
R. H. Bragg

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

136. HIGH-TEMPERATURE OXIDATION AND CORROSION OF MATERIALS — 340,000 — 01-3
D. P. Whittle

The effects of metallurgical and environmental variables on the surface degradation of materials in sulfur-containing atmospheres. The chemistry of sulfatic deposits and their influence on hot corrosion. Oxide stoichiometry changes in the presence of sulfur and transport studies in oxide solutions and their relationships to mechanisms of materials degradation. Active element additions to alloys and coatings to promote improved scale substrate adhesion; the nature of the scale/substrate interface. Multicomponent diffusion in coating/alloy systems and in oxide solid solutions.

137. REFRACTORIES PROJECT: PROCESSING; MECHANICAL PROPERTIES, AND CHEMICAL PROPERTIES — 180,000 — 01-3
L. C. De Jonghe, A. G. Evans, and D. P. Whittle

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

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division

138. CERAMIC INTERFACES 20,000 01-3
A. M. Glaeser

An experimental technique using local laser heating and/or melting to stimulate abnormal grain growth will be developed. The technique will permit the migration behavior of individual grain boundaries in a wide variety of materials to be investigated. The temperature and driving force dependence of the grain boundary migration rate in near-theoretical density Mg-doped Al_2O_3 will be determined using this technique and/or normal grain growth experiments.

139. EROSION-CORROSION WEAR PROGRAM 325,000 01-5
A. V. Levy

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

140. FAR INFRARED SPECTROSCOPY 195,000 02-2
P. L. Richards

Development of improved types of far infrared detectors, mixers and spectrometers. Use of advanced infrared techniques for the measurement of: the vibrational frequencies of molecules chemically adsorbed on metal surfaces, the infrared properties of solids with charge-density wave transitions, the far infrared spectra of electrons trapped on the surface of liquid helium, the infrared photoconductivity of impurities in semiconductors, the infrared radiation from dust clouds in our galaxy, and the infrared radiation left over from the creation of the universe.

141. EXPERIMENTAL SOLID-STATE PHYSICS AND QUANTUM ELECTRONICS 230,000 02-2
Y. R. Shen

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

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division

142. EXCITED QUANTUM FLUIDS IN SOLIDS — 150,000 — 02-2
C. D. Jeffries

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

143. TIME-RESOLVED SPECTROSCOPIES IN SOLIDS — 60,000 — 02-2
P. Y. Yu

Application of an optical system capable of measuring absorptivity, reflectivity, photoluminescence and light scattering spectra with time resolution of picoseconds to the study of the following phenomena: relaxation of photoexcited hot carriers via carrier-phonon interaction; decay of nonequilibrium phonon populations; temporal behavior of resonant raman spectra and hot luminescence, and transient phenomena involving defects and impurities in solids.

144. SUPERCONDUCTIVITY, SUPERCONDUCTING DEVICES, AND 1/f NOISE — 235,000 — 02-2
J. Clarke

Development of Superconducting Quantum Interference Devices (SQUIDS) for measuring voltages and fluctuations in magnetic fields and magnetic field gradients; quantum noise processes in Josephson junctions and SQUIDS; operation of SQUIDS as high frequency amplifiers. Use of SQUIDS in magnetotelluric measurements of the apparent resistivity of the earth's crust, use of SQUIDS to measure magnetic field gradient fluctuations at the earth's surface. Nonequilibrium superconductivity; enhancement of the superconducting energy gap and transition temperature by microwaves and phonons; quasiparticle charge relaxation in presence of magnetic impurities or a supercurrent; measurement of the electron-phonon relaxation times in aluminum, tin, and lead; generation of charge imbalance by temperature gradients.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division

145. THEORETICAL STUDIES OF THE ELECTRONIC PROPERTIES OF SOLID SURFACES — 40,000 — 02-3
L. M. Falicov

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

146. THEORETICAL SOLID-STATE PHYSICS — 60,000 — 02-3
M. L. Cohen

The major objective of the program is to explain the properties of solids using microscopic theory. The focus of the research has been on bulk and surface electronic properties of solids using pseudopotential techniques. Other areas of research include optical properties, superconductivity, surface and interface physics, band structure, pseudopotential theory, and structural properties of semiconductors and metals. A recent advance is the determination of crystal structure, lattice constant, bulk moduli, lattice vibrational frequencies, and crystalline phase transformation using the atomic number and atomic mass as the only input.

147. LOW TEMPERATURE PROPERTIES OF MATERIALS — 145,000 — 03-1
N. E. Phillips

The general objective of this program is to obtain low-temperature data, particularly heat-capacity data, that contribute to an understanding of the relations between atomic properties and the macroscopic properties of materials. The materials investigated include normal and superconducting metals, superfluids, dielectric solids, and magnetic materials. Heat capacity measurements are confined to temperatures below 25K because usually only in that region can various contributions be reliably separated. The temperature scale for the region from 0.06 to 25K is maintained on germanium thermometers and its relation to various "absolute" scales is well established. For temperatures from 0.06K to the mK region, γ-ray anisotropy and nuclear susceptability thermometers are being intercompared and used to calibrate various working thermometers.

LAWRENCE BERKELEY LABORATORY
Materials and Molecular Research Division

148. ELECTROCHEMICAL PROCESSES — 131,000 — 03-1
C. W. Tobias

This program is designed to advance the scientific foundations of electrochemical engineering, and to widen the range of useful applications of electrochemical influences of electrode geometry, surface potential, and ionic transport on the distribution of current on electrode macroprofiles. Gas-electrolyte-electrode interfaces: supersaturation, coalescence, and bubble separation phenomena. Nonaqueous ionizing media: thermodynamic and kinetic properties of electrode reactions which are not feasible in aqueous media.

149. HIGH TEMPERATURE THERMODYNAMICS — 131,000 — 03-3
L. Brewer

Characterization of the high-temperature chemical behavior of materials, particularly refractory ceramic materials, metals and gases. The high temperature thermodynamic properties are being determined through use of solid-electrochemical cells, solid-gas equilibria, and by X-ray and metallographic characterization of phase boundaries. The data are being used to test and improve chemical models capable of predicting the thermodynamic and elastic properties of high-temperature materials.

150. CHEMISTRY AND MATERIALS PROBLEMS ENERGY PRODUCTION TECHNOLOGIES — 220,000 — 03-3
D. R. Olander

Chemical and physical behavior of materials in environments characteristic of energy production devices, with major emphasis on fission and fusion reactors. Experiments are designed to develop insight into the mechanisms of the phenomena involved: the high temperature behavior of uranium dioxide, including transient vaporization, oxygen self-diffusion, thermal gradient migration of inclusions, and hydrogen solubility; molecular beam studies of gas-solid reactions, including hydrogen atom reaction with ceramic oxides and the silane cracking reaction; stress corrosion cracking of zircaloy; brine inclusion migration in salt.

151. PLASMA ENHANCED DEPOSITION OF THIN FILMS — 55,000 — 03-3
D. W. Hess

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

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Materials and Molecular Research Division

152. ELECTROCHEMICAL PHASE BOUNDARIES 150,000 03-3
R. H. Muller

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

153. SOLID STATE AND SURFACE REACTIONS 316,000 03-3
G. A. Somorjai

Studies of catalyzed surface reactions and of the atomic structure and chemical composition of solid surfaces and adsorbed monolayers. Kinetics and mechanisms of catalytic surface reactions on crystal surfaces at low and at high pressures. A combination of surface techniques is used: Auger electron spectroscopy, low energy electron diffraction, electron energy loss spectroscopy, molecular beam scattering, gas chromatography, and mass spectroscopy. Catalyzed hydrocarbon conversion reactions are studied. The building of new catalysts that are likely substitutes for the platinum metals are attempted by deposition of ordered metal monolayers on the surfaces of other metal single crystals and by the use of transition metal sulfides.

154. NUCLEAR MAGNETIC RESONANCE 132,000 03-3
A. Pines

Nuclear spin interactions and their use in developing new nmr techniques. Molecular properties of ordered condensed phases and effect of nuclear spin on chemical processes. Development of multiple quantum spectroscopy. Molecular behavior of organized matter, solids, liquid crystals, molecules absorbed on surfaces and molecules excited by light. Optical nuclear polarization and magnetic resonance of molecules in excited states.

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Livermore, California 94550

W. F. Krupke - Phone: (FTS) 532-5905 or 415-422-5905

155. HOT CORROSION STUDIES RELATED TO FOSSIL FUELS — $300,000 — 01-1
J. Truhan, O. Krikorian

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

156. OPTICAL MATERIALS RESEARCH — $260,000 — 02-2
M. Weber, A. Rosencwaig
C. Cline, H. Newkirk

Nonlinear optical properties of transparent materials subject to intense light beams and growth and spectroscopy of new laser materials. Intensity-dependent refractive index changes measured using time-resolved laser interferometry. Two-photon absorption at near-ultraviolet to near-infrared wavelengths detected using photoacoustic and photorefractive techniques. Dependence of spectroscopic and optical properties on material composition. Materials include oxide and fluoride glasses and crystals.

157. LASER-EXCITED FLUORESCENCE IN AMORPHOUS SOLIDS — $230,000 — 02-2
S. Brawer, M. Weber

Laser-induced fluorescence line narrowing and optical site selection spectroscopy to probe variations in local fields and electron-phonon coupling at paramagnetic ion sites in disordered solids. Simple and multicomponent oxide and fluoride glasses. Experimental spectra are compared with site-dependent fluorescence properties calculated from computer simulations of glass structure using Monte Carlo and molecular dynamic methods.

LAWRENCE LIVERMORE NATIONAL LABORATORY (continued)

158. SURFACE PHYSICS AND CHEMISTRY OF LASER INDUCED DAMAGE — $230,000 — 02-2
W. Siekhaus, W. Lowdermilk

Investigation of the fundamental physical and chemical processes determining the thresholds for laser-induced damage of transmitting optical materials and thin-film coatings. Studies of the relation between damage thresholds of the bulk and surfaces, dependence of damage thresholds on the physical structure of surfaces, effects of absorption of foreign atoms, surface chemical reactions, and migration of impurities. Polished crystalline and amorphous samples are cleaned by laser irradiation in a vacuum chamber and tested in situ using 1.06, 0.53 and 0.35 μm laser pulses. Multiphoton induced electron emission is monitored along with Auger analysis.

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

Measurement of D_2+T_2 chemical reaction rates in the solid and liquid phases by infrared spectroscopy. Measurement of D_2-T_2 rotational reaction rates by nuclear magnetic resonance. Engineering-type measurements on a DT-He^3 mixture phenomenon that halts the flow of gas into the cryostat. Study of frozen "super-ions" in solid T_2 using infrared spectroscopy. The D_2+T_2 gas phase kinetic experiments using mass spectroscopy. Solid thermal conductivity measurements using nuclear magnetic resonance. Optical absorption spectroscopy of trapped electrons in the solid.

Bailey
843-5893
John Browne
843-6162

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

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

160. THE EFFECT OF SELF-IRRADIATION ON STABILITY OF CERAMIC NUCLEAR WASTE — $210,000 — 01-4
F. W. Clinard, Jr., G. F. Hurley, D. E. Peterson, D. L. Rohr

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

161. RADIATION EFFECTS STUDIES FOR ADVANCED ENERGY TECHNOLOGIES — $310,000 — 01-4
D. M. Parkin, J. R. Cost
W. F. Sommer

800 MeV proton (LAMPF) irradiation of Al under cyclic stressing and proton irradiation effects in technologically important materials; interaction of radiation damage and mechanical damage; modeling of damage; microstructure development under pulsed irradiation; radiation effects in amorphous metals; atomic mobility in amorphous and crystalline metals.

162. MATERIAL DEFORMATION UNDER MULTIAXIAL LOADING — $263,000 — 01-5
S. S. Hecker, J. J. Petrovic, M. G. Stout, K. Staudhammer, D. L. Rohr

Multiaxial deformation of aluminum, aluminum alloys, titanium, brass and 304 stainless steel; tube testing; yield surfaces and stress-strain relations under multiaxial loading; effects of stress path changes; hydrogen effects in multiaxially loaded titanium; substructural evolution with strain, strain state and strain rate; deformation-induced transformation in 304 stainless steel; brittle fracture of Al_2O_3, Si_3N_4, SiC and ZrO_2 under multiaxial stresses; mixed-mode brittle fracture; Weibull statistical fracture theory; fracture toughness of ceramics.

163. CTR RELATED TRITIUM CHEMISTRY RESEARCH ASSOCIATED WITH THE BREEDER BLANKET AND CONTAINER MATERIALS — $182,000 — 03-2
D. H. W. Carstens, J. L. Anderson

Equilibrium pressure measurements of tritium, deuterium, and protium over lanthanum metal and over La_5Ni, a low melting, liquid-metal tritium getter. Determination of Sieverts' constants of hydrogen isotopes in the metal and in the alloy. Development of a scheme for recovering tritium from the alloy using an intermediate amalgum.

Physics Division
T. F. Stratton - Phone: (FTS) 843-4117 or 505-667-4117

164. MATERIALS RESEARCH ON THE LOS ALAMOS SPALLATION NEUTRON SOURCE — $850,000 — 02-1
R. N. Silver, A. Soper, J. Eckert, A. Taylor, J. Goldstone, P. Vergamini, P. Seeger, A. Larson, C. E. Olsen

Materials research and neutron scattering instrument development to utilize the new WNR/PSR pulsed spallation neutron source. Inelastic neutron scattering studies of metal hydrides, chemical spectroscopy, and surfaces. Neutron diffraction studies of molecular liquids, amorphous materials, powders, and single crystals. Development of novel time of flight neutron scattering instrumentation.

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

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

166. THERMOPHYSICAL PROPERTIES OF MATERIALS — $100,000 — 02-2

J. C. Wheatley, H. K. Collan, A. Migliori, G. W. Swift, A. Fartash, J. J. Haucke, J. Helfrich, T. J. Hofler, Y. Maeno

Properties of liquids working in heat engines; scientific qualities of Stirling and Stirling-Malone heat engines, heat pumps, and refrigerators using propylene near room temperature, helium isotopes at low temperatures, and liquid water and NaK at higher temperatures; properties of the required "second thermodynamic media", novel approaches to making the liquid medium go through its thermodynamic cycle. Helium isotope heaT engines which cross the critical region. Heat transfer by diffusive conduction and gravitational convection in very dilute solutions of ^{3}He in superfluid ^{4}He. Novel processes of heat transfer in ^{3}He-^{4}He solutions near the tricritical point. Properties of gaseous hydrogen isotopes at low temperatures.

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

167. ELASTIC WAVE SCATTERING AND QUANTITATIVE FLAW IDENTIFICATION — $157,000 — 01-5

J. E. Gubernatis — 843-6727
W. M. Visscher
G. A. Baker, Jr.

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

168. LOS ALAMOS EQUATION OF STATE LIBRARY — $260,000 — 02-3

J. Abdallah, R. C. Albers, B. I. Bennett, W. F. Huebner, J. D. Johnson, G. I. Kerley, S. P. Lyon

Maintain a computer-based library of equations of state (EOS) and other material properties such as opacities, and electrical and thermal conductivities for application to energy programs. Survey current user requirements and calculate or acquire and evaluate the needed data. Store data in tabular form suitable for use in realistic hydrodynamic code calculations and other applications. Distribute data to users on magnetic tape in a universal computer format. Apply theories of solids, liquids, gases, plasmas, and mixtures to generation of EOS data. Develop new theoretical methods when existing theories and experiments are insufficient to satisfy user requirements.

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

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

169. DOE FACILITY USERS PROGRAM $105,000 01-1
W. E. Felling

This project supports collaborative work between university researchers and national laboratories; one program involves apparatus at ORNL such as the high voltage electron microscope and the analytical electron microscope; the second program involves the National Synchrotron Light Source at BNL.

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Oak Ridge, Tennessee 37830

Metals and Ceramics Division -01-
J. R. Weir, Jr. - Phone: (FTS) 624-4065 or 615-574-4065
C. J. McHargue - Phone: (FTS) 624-4344 or 615-574-4344

170. THEORETICAL STUDIES OF METALS AND ALLOYS $400,000 01-1
J. S. Faulkner, W. H. Butler, G. S. Painter, G. M. Stocks, H. Winter

Local density formalism (LDF) combined with cluster program and layer KKR program to study electronic states of surfaces and energetics such as binding energy of adsorbates, surface molecular dissociation, and chemical properties of reaction intermediates as related to catalysis; small molecular clusters, absorption of O on Al and O, S on Ni; band theory of metals, alloys and compounds, self-consistent CPA treatment of random substitutional solid solutions, residual resistivity, comparison with results of photoemission experiments, extension of theory beyond CPA; calculation of binding energies and phase stability in alloys; superconducting transition temperature and H_{C2} and phonon line width; phonon contribution to lattice conduction in Nb, Mo, and Pd; electron-phonon and electron-electron enhancement effects in metals; cohesive energy and magnetic moment of Fe.

171. HIGH-TEMPERATURE STRUCTURAL CERAMICS $500,000 01-1
V. J. Tennery, C. B. Finch, G. W. Clark, C. S. Yust, P. F. Becher

Synthesis, fabrication, characterization, and evaluation of hard structural ceramics including materials from TiB_2-Ni, TiB_2-CrB_2-Ni, other boride and carbide systems with objective of determining compositional and microstructural requirements for severe erosive and corrosive environments; preparation and evaluation of directionally solidified eutectics in TiB_2-oxide systems; mechanisms for increasing fracture energy and high-temperature strength of selected oxide and carbide structural ceramics; growth of single crystals of β'-sialon; transformation toughening in Al_2O_3-ZrO_2, HfO_2, ion beam modification of ceramic surfaces.

172. STRUCTURE OF COAL $125,000 01-1
L. A. Harris, O. C. Kopp

TEM, SEM, microprobe, optical and infrared petrography of microporosity and micromineralogy of coal macerals; correlation of coal rank with micro-structure; characterization of secondary minerals; anthracite, bituminous, sub-bituminous, and channel coals; in situ studies of maceral-mineral and maceral-maceral reactions using HVEM.

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

173. X-RAY SCATTERING RESEARCH $400,000 01-1
C. J. Sparks, B. S. Borie, G. E. Ice, H. L. Yakel

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

174. HIGH VOLTAGE AND ANALYTICAL ELECTRON MICROSCOPY $325,000 01-1
J. Bentley, A. P. Fisher, E. A. Kenik, E. H. Lee

Development and application of analytical transmission microscopy and HVEM to determine the microstructure and microchemistry of solids; weak-beam dark-field studies of precipitates in irradiated alloys; lattice imaging of two-phase interfaces; SAES and EELS of internally oxidized refractory metal alloys; structure of long-range ordered alloys; in situ deformation, oxidation, and hydriding studies in the 1-MeV microscope; grain boundary phases in structural ceramics; structure of metallic glasses; standardless EELS analysis.

175. DEFORMATION AND MECHANICAL BEHAVIOR OF STRUCTURAL MATERIALS $470,000 01-2
M. H. Yoo, K. Farrell, J. C. Ogle, J. Schneibel, C. L. White

Experimental and theoretical studies of effects of impurities and interfaces on deformation and fracture of Ni, Fe-Ni, Ni-Cr, Fe-Ni-Cr alloys; grain boundary cavity nucleation and growth; hydrogen effects; segregation of impurities to grain boundaries and creep cavities; dynamic recrystallization; small-angle neutron scattering studies of cavity growth during creep and fatigue in nickel.

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

Defect interactions during diffusion and during growth of surface layers; kinetics of sulfur reactions with Fe-base alloys, definition of the electronic-ionic defect structure of FeS; diffusion in sulfur-doped oxides; stress generation and relaxation in sulfide scales; sulfur attack of ion implanted Fe-base alloys. Theoretical treatment of vacancy and interstitial diffusion in compounds having high defect concentrations.

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

177. PHYSICAL PROPERTIES RESEARCH $300,000 01-3
D. L. McElroy, J. P. Moore, R. K. Williams

Development and application of measurement methods for physical property studies from 4.2 to 2600 K; correlation of electronic energy transport through the Lorenz constant; phonon scattering by electrons and defects in refractory metals and alloys (V, Nb, Ta, Cr, Mo, W, Pd) and transition metals (Fe, Ni, Cr); phonon-phonon scattering in insulating solids, effect of cation-anion mass ratio, grain boundaries and crystal structure; properties of LRO alloys.

178. AMORPHOUS AND METASTABLE MATERIALS $500,000 01-3
C. C. Koch, A. DasGupta, D. S. Easton, D. M. Kroeger

Amorphous superconductors based on Mo, Nb, La, and Re with other transition metals and/or metalloids; influence of inhomogeneous deformation on structure and fluxoid pinning in amorphous superconductors; stability of binary and ternary metallic glasses; critical cooling rates for glass formation; preparation techniques by arc-hammer, melt spinning, and electron-beam vapor deposition; mechanical properties of metastable materials; low temperature specific heat; small-angle x-ray and TEM studies of defect structure and phase separation in Mo-Ru-B.

179. RADIATION EFFECTS $1,300,000 01-4
L. K. Mansur, W. A. Coghlan, K. Farrell, E. A. Kenik, M. B. Lewis, N. H. Packan

Neutron damage in pure metals and alloys irradiated in ORR, HFIR, and EBR-II, effect of alloying additions, impurities and microstructure on void nucleation and growth; phase stability under irradiation; damage simulation studies using multiple ion beams (heavy and dual light ions), relationship between ion and neutron damage, effect of helium and other gases on nucleation and growth of voids and interstitial loops; irradiation creep simulation; theoretical studies of void and loop nucleation and growth, solute-defect interactions, irradiation creep HVEM irradiations; Al, Zr, Ni and alloys, stainless steels, LRO alloys, ferritic alloys.

180. WEAR OF CERAMICS $150,000 01-5
C. S. Yust

Analysis of wear rates and microstructural damage in TiB_2, ZrB_2, WC and SiC; TEM study of damage process; effect of environment, loading conditions, crystallography.

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

181. FUNDAMENTAL STUDIES IN WELDING $330,000 01-5
G. M. Goodwin, S. A. David, J. M. Vitek

Control of weld microstructure through control of solidification parameters; composition, distribution, and stability of micro-phases; microstructure of laser-produced welds; modeling of solidification processes; austenitic steels.

182. STUDIES IN NONDESTRUCTIVE EVALUATION $100,000 01-5
W. A. Simpson, C. V. Dodd

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

Boatner — wed X5492

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-
M. K. Wilkinson - Phone (FTS) 624-6151 or 615-574-6151
F. W. Young, Jr. - Phone (FTS) 624-5501 or 615-574-5501

2.1

183. INTERATOMIC INTERACTIONS IN CONDENSED SYSTEMS — $1,290,000 — 02-1 ✓
R. M. Nicklow, J. W. Cable,
H. R. Child, W. C. Koehler,
H. A. Mook, R. M. Moon,
H. G. Smith, N. Wakabayashi,
K. Werner

Inelastic neutron scattering studies of phonons, magnons and single particle excitations in condensed matter; elastic and inelastic scattering of polarized and unpolarized neutrons by magnetic materials; lattice dynamics of $CePd_3$, LaB_6, SmS, and martensitic alloys; magnetic excitations in UAl_2, $CePd_3$, Gd at high temperatures, and Er; magnetic structures of Nd and MnP; magnetic form factors of mixed valence materials; structures of composition modulated systems.

184. PROPERTIES OF DEFECTS, SUPERCONDUCTORS AND HYDRIDES — $810,000 — 02-1 ✓
R. M. Moon, J. W. Cable,
H. R. Child, W. C. Koehler,
H. A. Mook, R. M. Nicklow,
L. Pintschovius, H. G. Smith,
N. Wakabayashi, G. D. Wignall

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

185. PHYSICAL PROPERTIES OF CERAMICS — $325,000 — 02-2
E. Sonder, Y. Chen,
R. R. Gonzalez, F. A. Modine,
R. A. Weeks

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

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

186. HIGH TEMPERATURE PROPERTIES OF CARBIDES AND NITRIDES — $215,000 — 02-2
F. A. Modine, G. R. Gruzalski, T. W. Haywood, W. R. Major

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

187. SOLID ELECTROLYTES AND SUPERIONIC CONDUCTIVITY — $260,000 — 02-2
J. B. Bates, N. Bjerre, G. M. Brown, W. E. Brundage, N. J. Dudney, H. L. Engstrom, B. C. Larson, J. C. Wang

Mechanisms of high ionic conductivity in the beta- and beta"-aluminas; effects of impurities and crystal growth conditions on conductivity; effect of water intercalation on ion transport in the beta- and beta"-aluminas; thermodynamics and kinetics of water intercalation; structural and dynamical properties of ionic conductors; techniques include measurements of electrical conductivity and dielectric constant, Raman scattering, infrared absorption, neutron and x-ray diffraction and x-ray diffuse scattering; experimental results interpreted and correlated by means of model calculations.

188. PHYSICAL PROPERTIES OF SUPERCONDUCTORS — $455,000 — 02-2
S. T. Sekula, B. R. Appleton, D. K. Christen, H. R. Kerchner, J. R. Thompson, C. W. White

Studies of fluxoid lattice arrays, flux flow, flux creep, fluxoid defect interactions, and anisotropy in Nb-, V-, and Ta-base alloys and superconducting compounds with A15 and B1 crystal structures; small-angle neutron scattering by equilibrium and metastable fluxoid lattice configurations in superconductors; dc magnetization, ac magnetic permeability, critical-current and normal-state electrical transport; ion damage, ion implantation, and ion backscattering in bulk and thin-film superconductors; laser annealing studies of superconductors.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

189. PREPARATION AND CHARACTERIZATION OF RESEARCH MATERIALS — $635,000 — 02-2
L. A. Boatner, W. E. Brundage, Y. K. Chang, G. R. Gruzalski

Growth and characterization of high-quality single crystals of metals, alloys, and insulators; float-zone and tri-arc growth of crystals of A15 compounds such as V_3Si, V_3Ge, Ti_3Au, and Ti_3Pt; arc-fusion and flux growth of crystals of high temperature materials (WC, Y_2O_3, MgO, CaO, SrO); flux growth of single crystals of fast-ion conductors (β-alumina, β"-alumina); growth of perovskite-structure oxides ($K_{1-x}Li_xTaO_3$, $KTaO_3$, $KTa_{1-x}Nb_xO_3$) and semiconducting oxides for photoelectrochemical cell electrode investigations; Czochralski and float-zone growth of crystals of Fe-Ni-Cr alloys (i.e., stainless steels); growth of refractory metal crystals (Ti, V, Zr, Nb, Ta, W, Ir, Re) using the electron-beam float-zone technique. RF induction float-zone growth of transition metal carbides.

190. PHOTOPHYSICAL PROCESSES OF SOLAR ENERGY CONVERSION — $665,000 — 02-2
R. F. Wood, J. W. Cleland, L. S. Darken, J. Fletcher, R. B. James, G. E. Jellison, B. C. Larson, D. H. Lowndes, J. Narayan, G. van der Leeden, R. D. Westbrook, C. W. White, R. T. Young

Effects of point defects, defect clusters, dislocations, grain boundaries, stacking faults, and chemical impurities on electrical and optical properties of single crystal and polycrystalline Si; thermal neutron transmutation, diffusion, and ion implantation doping experiments for fabrication of p-n junctions; fabrication of high efficiency Si and GaAs solar cells by laser techniques; thermal and laser annealing of lattice damage in Si and GaAs; laser-induced recrystallization of amorphous layers; electrical, optical (including infrared and luminescence spectroscopy), transmission electron microscopy, electron paramagnetic resonance, x-ray scattering, surface photovoltage, secondary ion mass spectrometry, and Rutherford ion backscattering property measurements; grain boundary compensation in polycrystalline Si; dopant concentration profiles, deep-level transient spectroscopy, and absolute quantum efficiency measurements; fabrication of test solar cells; solar cell modeling; factors affecting degradation of solar cell conversion efficiency under single sun and concentrator conditions; laser-induced grain growth in polycrystalline materials; graphoepitaxy and thin-film deposition on prepared substrates; chemical vapor deposition of Si and GaAs on low-cost substrates.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

191. FUNDAMENTAL ASPECTS OF METAL FRACTURE — $340,000 — 02-2
S. M. Ohr, S.-J. Chang, J. A. Horton, J. Narayan, T. S. Noggle

Experimental and theoretical investigations to relate phenomena of continuum fracture mechanics to microscopic physical phenomena occurring at a crack tip; *in situ* transmission electron microscope observations of crack propagation in aluminum, copper, nickel, molybdenum, niobium, tungsten, stainless steel, magnesium oxide, and niobium oxide; crack propagation in metals containing helium bubbles; distribution of dislocations in the plastic zone ahead of the crack tip in metals and ceramics; cyclic deformation; ductile-brittle transition in bcc metals; dislocation theory of J-integral; theory of the plastic zone with a dislocation-free zone.

192. SCATTERING OF SYNCHROTRON RADIATION — $105,000 — 02-2
B. C. Larson, R. M. Nicklow, T. S. Noggle, G. T. Trammell, C. W. White

Defect structures and defect correlations in solids; x-ray diffuse scattering; transient effects associated with pulsed laser annealing; energy resolved x-ray scattering; quasi-elastic scattering.

193. THEORY OF CONDENSED MATTER — $960,000 — 02-3
J. F. Cooke, J. H. Barrett, H. L. Davis, L. J. Gray, T. Kaplan, P-A. Lindgård, S. H. Liu, M. E. Mostoller, O. S. Oen, A. K. Rajagopal, M. Rasolt, M. T. Robinson, J. C. Wang, R. F. Wood

Theory of laser annealing, laser-induced diffusion, and nonequilibrium solidification in semiconductors; superionic conductivity and solid electrolytes; computer simulation of radiation damage and sputtering; radiation damage analysis procedures; correlation of neutron damage with ion bombardment; radiation emitted by channeled electrons and positrons; reflection of light atoms from surfaces; surface studies with backscattered ions; development of LEED theory and interpretation of LEED data; crystallography of laser-annealed semiconductors; surface vibrations and relaxation; correlation contributions to surface energy; optical potential for electron spectroscopies; theory of angular effects in photoemission and Auger emission of electrons from surface regions; electron screening and phonon spectra; lattice dynamics of high T_c superconductors; magnetism in transition metals; Brillouin zone integration; Heisenberg spin systems; metal-hydrogen interactions; high temperature oxides and carbides; lattice vibrations in disordered alloys; coherent potential approximation; vibrational properties around substitutional impurities in insulators; neutron scattering from molecular-like impurities in crystals; electronic properties of rare-earth and actinide compounds; band structure calculations for metals and insulators.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

194. LOW TEMPERATURE RADIATION EFFECTS — $230,000 — 02-4
R. R. Coltman, Jr., C. E. Klabunde

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

195. X-RAY DIFFRACTION AND ELECTRON MICROSCOPY — $535,000 — 02-4
B. C. Larson, J. F. Barhorst, J. Narayan, T. S. Noggle, S. M. Ohr, J. Fletcher, J. A. Horton

Structure of intrinsic and induced defects in solids; transmission electron microscopy; x-ray diffuse scattering; x-ray topography; defect clusters resulting from fast neutron and ion irradiations of Cu, Ni, Au, Ag, Si, Nb, and stainless steel; pulsed laser annealing; defects associated with laser and thermal processing of pure and ion-implanted semiconductors; cell structure in doped semiconductors; grain boundaries in semiconductors; defects in high temperature oxides; anisotropic elastic theory of dislocation loops; computer simulation of electron microscopy images; calculation of diffuse scattering from dislocation loops and solute precipitates; theory of interactions of electrons and x-rays with defects in solids.

196. NORMALIZATION OF ION AND NEUTRON DAMAGE — $100,000 — 02-4
T. S. Noggle, B. R. Appleton, O. S. Oen, D. B. Poker, J. M. Williams

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

197. GASES IN METALS — $215,000 — 02-4
D. B. Poker, J. M. Williams, R. R. Coltman

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

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

198. SURFACE PHYSICS AND CATALYSIS $665,000 02-5
L. H. Jenkins, H. L. Davis,
J. R. Noonan, S. Overbury,
G.-C. Wang, J. F. Wendelken,
C. W. White, D. M. Zehner

Studies of the crystallographic and electronic structure of clean and adsorbate-covered metal and semiconductor surfaces with emphasis on surfaces which either reorder or have interplanar spacings different from those of the bulk; combined techniques of low energy electron diffraction (LEED), positive ion crystallography of surfaces (PICS), low energy ion scattering spectroscopy (ISS), polarized low energy electron diffraction (PLEED), photoelectron spectroscopy (PES), and computer simulations for surface crystallography studies; LEED, PES, and Auger electron spectroscopy (AES) combined with in situ laser annealing of semiconductors; lineshape analysis of Auger spectra; LEED, AES and x-ray photoelectron spectroscopy (XPS) studies of both clean and adsorbate-covered surfaces of metals and intermetallic compounds; vibronic structure of adsorbates examined by high resolution electron energy loss spectroscopy (EELS) examination of surface electronic and geometric structures with respect to solid state aspects of heterogeneous catalysis.

199. ION BEAM ANALYSIS AND ION IMPLANTATION $730,000 02-5
B. R. Appleton, J. H. Barrett,
G. M. Beardsley, L. H. Boatner,
Y. K. Chang, R. J. Culbertson,
J. Fletcher, O. W. Holland,
E. J. Kelly, B. C. Larson,
C. J. McHargue, H. Naramoto,
J. Narayan, T. S. Noggle,
O. E. Schow III, B. W. Stritzker,
C. W. White, J. M. Williams,
S. P. Withrow, D. M. Zehner

Continued development of positive ion crystallography of surfaces (PICS) technique; application of PICS to reordered and relaxed metal surfaces and to metastable semiconductor surfaces formed by pulsed laser annealing; fundamental studies of laser annealing; studies of high-speed nonequilibrium crystal growth; investigations of segregation, constitutional supercooling, substitutionality, and solute trapping effects, and determination of mechanisms limiting maximum substitutional concentrations of ion implanted impurities subjected to pulsed laser processing; study of supersaturated substitutional alloys, new metastable phases and amorphous alloys fabricated by ion beam and pulsed laser processing; fundamental investigations of ion beam and laser induced materials interactions; applications of ion implantation doping and pulsed laser processing to studies of corrosion/catalysis mechanisms, to reduction of friction and wear of metal surfaces, to improvement of wear, hardness and structural properties of ceramics, to improvements in high temperature materials, and to the fabrication of high transition temperature superconductor compounds from thin film composites; fundamental studies of ion-solid interactions (particularly ion channeling) with applications to materials analyses.

OAK RIDGE NATIONAL LABORATORY
Solid State Division -02-

200. RADIOACTIVE WASTE STORAGE — $335,000 — 02-5
L. A. Boatner, M. M. Abraham,
P. G. Huray, M. Petek,
B. C. Sales

Evaluation of lanthanide orthophosphates (i.e., analogs of monazite) as primary containment forms for α-active actinide wastes; growth of actinide doped single crystals; determination of valence states and site symmetries of actinide and other impurities using electron paramagnetic resonance, x-ray, optical, and Mössbauer techniques; leaching of radioactive ions from orthophosphates under various conditions; use of a molten urea process for the production of orthophosphate powders with controlled particle sizes; compaction and microstructural characterization of hot-pressed or cold-pressed, sintered orthophosphate bodies; studies of α-particle induced radiation effects in lanthanide orthophosphate compounds. Characterization of borosilicate glass waste forms and SYNROC phases.

201. RESEARCH AND DEVELOPMENT - ISOTOPE RESEARCH MATERIALS PREPARATION — $320,000 — 02-5
E. H. Kobisk, W. S. Aaron,
H. L. Adair, P. R. Kuehn,
T. C. Quinby, J. A. Setaro,
R. D. Taylor

Research and development in preparation techniques involved with isotope-containing samples in the form of ultra-thin films (supported and self-supported), wires, rods, cast shapes, alloys, ceramics, cermets, distilled metals, inorganic and refractory compounds, matrix-dispersed materials, and liquids; techniques of preparation include vapor deposition, ion sputtering, rolling, chemical vapor deposition, liquid phase and conventional sintering, hot pressing, isostatic pressing, electrodeposition, molecular plating, zone refining, reactive and ordinary spray calcination, inorganic chemical methods; characterization of prepared research samples includes x-ray and electron diffraction, electron microscopy (TEM and SEM), microprobe studies, differential thermal analysis, thermal conductivity determinations, resonating crystal thickness monitoring, x-ray fluorescence, radiation counting (low geometry and absolute), and microweighing; phase diagram determinations for compounds and metals; all development efforts equivalent for stable and light and heavy radioactive materials.

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Chemistry Division -03-
O. L. Keller - Phone: (FTS) 624-4987 or 615-574-4987

202. CHEMICAL STRUCTURE OF ENERGY RELATED MATERIALS — $870,000 — 03-1
W. R. Busing, G. M. Brown, G. J. Bunick, C. K. Johnson, E. Johnson, A. H. Narten, W. E. Thiessen, R. Triolo

Atomic and molecular arrangements in crystals and in liquids determined by neutron and x-ray diffraction studies; atom-atom pair correlation functions for liquids; particle size distribution function in liquids; small-angle neutron scattering; development of synchrotron radiation facilities. Advancement of computational methods for solving and refining crystal structures; dynamic corrections to neutron scattering intensities; improvement of statistical mechanics for understanding molecular fluids and for extrapolating their physical properties; use of intermolecular potentials to interpret the conformation of molecules in crystals and liquids; development of a graphics display for presenting structures. Materials studied include liquid extracts of coal, superionic conductors for use in storage batteries and fuel cells, alloys with interesting thermal properties, hydrocarbon fuels, compounds which are potential catalysts for hydrogenation and hydrogen production, and minerals stable at high temperatures and pressures in the mantle of the earth.

203. HIGH TEMPERATURE CHEMISTRY AND THERMODYNAMICS OF STRUCTURAL MATERIALS — $600,000 — 03-2
C. E. Bamberger, J. Brynestad, J. D. Redman, G. M. Begun

The thermodynamics and kinetics of formation/decomposition of microphases (carbides, nitrides) in high temperature steels are being investigated because such phases appear to be important in the corrosion and strength of steels. Studies are being completed of the high-temperature permeation of tritium through metals and alloys which are candidates for building steam generators for fusion reactors. Emphasis of the program is shifting toward the synthesis and characterization of high temperature materials (e.g., borides, carbonitrides) which may have multiple technological applications. Part of the program is devoted to synthesis and characterization of crystalline host materials intended for immobilizing radioactive fission product elements in nuclear waste that may come in contact with aqueous environmental media. One important feature of the approach to the synthetic chemistry is the correlation on the basis of theory and systematics of the physical, chemical, and structural properties of the newly developed materials.

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

204. PHYSICAL CHEMISTRY OF MOLTEN SALTS IN ENERGY UTILIZATION — $155,000 — 03-3
J. Braunstein, C. E. Vallet

Electrochemical relaxation, scanning electron microscopy and thermodynamics of irreversible processes are applied to characterize ion transport via diffusion and electromigration in molten salts and across interfaces between electrolytes and metals or semiconductors in high temperature systems.

205. LOCALIZED CORROSION AND STRESS CRACKING PHENOMENA RELATED TO ENERGY TECHNOLOGIES — $485,000 — 03-3
F. A. Posey, A. L. Bacarella, G. M. Brown, E. J. Kelly, A. A. Palko

Application of electrochemical methods coupled with ion implantation/Rutherford backscattering techniques to basic studies of mechanisms of corrosion reactions occurring in localized attack of metals (titanium, vanadium, etc.); investigation of properties of precisely-defined surface alloys (Ti-Pt, Ti-Mo, Ti-V, etc.); kinetics of coupled active-passive electrochemical systems; effects of soluble redox systems [Ti(IV)/Ti(III), V(IV)/V(III)/V(II), etc.] on localized corrosion of titanium; hydrolysis and speciation effects on kinetics of interfacial reactions in concentrated aqueous electrolytes encountered in localized corrosion; effect of alloy composition and temperature on pitting of titanium alloys as a function of the medium.

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

206. THERMODYNAMICS OF ENERGY RELATED SYSTEMS — $235,000 — 03-2
T. B. Lindemer, E. C. Beahm, T. M. Besmann

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

207. CHEMICAL ENGINEERING RESEARCH — $235,000 — 03-2
J. S. Watson, R. E. Barker, S. D. Clinton

Fundamental measurement and evaluation of material properties and behavior important to chemical processes; development and evaluation of techniques for characterization and physical removal of solid materials from fluids. Study of electrostatically enhanced deep-bed filtration techniques for removing submicron solid particles from gases and nonconducting liquids. Physical property measurements and correlations of organic mixtures similar to those produced and used in coal conversion processes.

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208. METAL-INSULATOR-SEMICONDUCTOR PHOTOVOLTAICS — $120,000 — 01-1
J. E. Garnier, L. C. Olsen

Effects of physical and chemical structure on the photoelectric behavior of metal-insulator-semiconductor devices. Characterization of thin film and interfacial structures, theoretical modeling of device characteristics, and correlation to fabrication parameters; Auger and ESCA surface analysis techniques and ellipsometry. Photoresponse, electrical transport measurements, sheet resistance, optical and IR spectroscopic analysis. Studies conducted on Al-Si and Au-Si devices.

209. PHOTOELECTROCHEMICAL PROPERTIES OF SOLAR MATERIALS — $90,000 — 01-1
R. Wang

Effects of crystal structure, microstructure and composition on the photoelectrochemical behavior of semiconductors and semiconducting films in liquid electrolytes. Study the anodic dissolution of metal oxides, doping of metal sulfides and passivation of grain boundaries in polycrystalline Si; electronic and photoelectrochemical properties of anodic films on amorphous alloy surfaces; degradation and corrosion of photoelectrodes; and surface modification for enhanced stability and efficiency.

210. SPUTTER-DEPOSITED AMORPHOUS SILICON FOR SOLAR APPLICATIONS — $85,000 — 01-1
P. M. Martin and W. T. Pawlewicz

Influence of H content and Si-H bonding on optical and electrical properties of sputter-deposited Si:H alloys; Si-H reaction kinetics during film growth; applications to photovoltaic solar cells, thin film coatings and multilayer dielectric stacks; optical and IR spectroscopic techniques, electrical transport measurements, gas evolution analysis; photoconductivity, x-ray fluorescence and x-ray diffraction.

PACIFIC NORTHWEST LABORATORY (continued)

211. EFFECT OF COAL MICROSTRUCTURE ON PROPERTIES $85,000 01-1
J. M. Lytle and J. L. Daniel

Grinding coal at controlled temperature, pressure and atmosphere conditions. Determination of rates of grinding and gas evolution during grinding. Quantitative characterization of the coal particles produced by grinding to determine microstructure, morphology, composition, size distribution, shape and petrography, and correlation of the particle properties with bulk properties. Study of modes and mechanisms of grinding by controlled grinding and in-situ scanning/electron microscope fracture experiments.

212. FUNDAMENTAL MECHANISMS OF STRESS CORROSION AND CORROSION FATIGUE $210,000 01-2
R. H. Jones, M. T. Thomas, S. M. Bruemmer, D. R. Baer

Investigations of the mechanisms controlling intergranular and transgranular stress corrosion and corrosion fatigue cracking of iron, iron-chromium-nickel and nickel-based alloys in gaseous and aqueous environments. Computer modeling and experimental measurements of surface and grain boundary segregation of S, P, Sb, C, N, and O in Fe and Ni as a function of time, temperature, and bulk concentration. Relationships between grain boundary chemistry, fracture thresholds of Fe and Ni in aqueous solutions are being studied. Effect of plastic strain and various gaseous environments (H_2S, Cl, NH_3) on the quantity and distribution of surface adsorbates is being studied by Auger Electron Spectroscopy using an in-situ straining stage.

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

Investigate the mechanisms controlling the high temperature corrosion of sputtered-deposited fine-grained materials. Oxidation and sulfidation studies of stainless steel in CO-CO_2 and CO-CO_2-H_2S gaseous environments at 800-1000°C, and hot corrosion studies on $Fe_{39}Co_{27}Cr_{22}Al_9Ni_3Y_1$ covered with Na_2SO_4 in a SO_2-O_2 atmosphere at 650-800°C. Use SEM, TEM, micro-focus x-ray diffraction and mechanical tests to determine the effect alloy grain size, alloying additions, and gaseous environment have on scale microstructure, scale adherence and scale cracking behavior. Employ AES, XPS, and nuclear microprobe measurements to examine changes in the diffusion and chemistry of elements in the alloy surface region, and determine the sequence of events that leads to accelerated corrosion.

PACIFIC NORTHWEST LABORATORY (continued)

214. LEACHING OF GLASS AND CERAMICS $90,000 01-3
G. L. McVay, L. R. Pederson, C. Q. Buckwalter

Mechanistic investigations of glass and crystalline ceramic interactions with aqueous solutions. Primary emphasis is upon the elemental interactions in the reaction layer (region between unaffected bulk material and the solution). Research areas include: surface potential measurements, radioactive tracer diffusion measurements, isotopic water reactions coupled with Rutherford backscattering and nuclear microprobe analyses, resorption kinetics, solution analyses, pH and oxygen level effects, and surface and near surface analyses using primarily Raman, ESCA and SIMS coupled with ion milling. Major goal is development of a predictive model for leaching.

215. RADIATION EFFECTS ON METALS $480,000 01-4
E. P. Simonen, J. L. Brimhall, H. E. Kissinger
L. A. Charlot, C. H. Henager, Jr., E. R. Bradley

Evaluation of radiation damage mechanisms in metals using heavy-ion, light-ion, neutron and electron bombardment; pulsed heavy and light-ion irradiations; in-situ irradiation creep testing; irradiation effects on creep, recovery, recrystallization, defect microstructures; interactions between substructure and irradiation damage; effects of the primary irradiation damage state on amorphous and crystalline phase stability; materials characterization using scanning transmission electron microscopy, microchemical analysis, x-ray diffraction, positron annihilation, rate theory evaluation of point defect bias parameters, migration and interaction energies; computer simulation of irradiation-induced microstructures; modeling of irradiation-affected dislocation mobility; studies of nickel, nickel alloys, pure bcc refractory metals, amorphous metals, ordered intermetallic compounds.

216. RADIATION DAMAGE IN CERAMICS 376 $110,000 01-4
G. J. Exarhos, W. J. Weber X0092

Structural and microstructural studies of ion-induced radiation damage in nonmetallic solids. Stoichiometric materials are subjected to external alpha bombardment from actinide sources or incur internal alpha-recoil damage from actinide doping. Characterization of the damage state and kinetic studies of damage in-growth and annealing utilizing x-ray diffraction, electron microscopy, sample density determinations, optical absorption, and vibrational Raman scattering measurements. Studies involving cubic oxides and fluorides, amorphization in rare earth silicates and phosphates, and theoretical model testing of mechanisms for damage in-growth and annealing are emphasized.

PACIFIC NORTHWEST LABORATORY (continued)

217. SPUTTERING PARAMETER INFLUENCES ON MATERIAL STRUCTURE AND BEHAVIOR — $180,000 — 01-5
E. D. McClanahan and W. T. Pawlewicz

Research on the process of high-rate sputtering to permit characterization and definition of the influence of sputtering parameters on the structure and behavior of sputter-deposited metallic and insulator materials. Study areas for metals (Mo and rare earth-transition metal alloys) include investigation and modeling of the parameters which influence the incorporation of gases (Kr, H_2 and CO) during sputter deposition, and investigation of relationships between structure, properties and thermal stability of metals containing significant quantities of gases. Study areas for insulators (ZrO_2) include stoichiometry, structure, properties, adherence to metallic substrates and controlled deposition at high rates. Materials characterization includes x-ray fluorescence and diffraction, metallography, SEM, TEM, thermal gas evolution analysis, electrical and optical property measurement, gas chromatography, calorimetry and differential thermal analysis. Particle energy and mass are analyzed during deposition.

218. OPTICAL LASER MATERIAL STUDY — $125,000 — 02-2
J. S. Hartman, J. W. Griffin, L. S. Dake, L. R. Pederson

Research on adhesion mechanisms at the silver/substrate interface in new second surface mirrors and after exposure to terrestrial environmental stresses (temperature, humidity, UV radiation): preparation and evaluation of mirrors as a function of (1) substrate material (simple crystalline: quartz; amorphous: fused silica; and complex: soda-lime silicate glass); (2) substrate preparation (abrasion, chemical cleaning, sputter etch): and (3) silver deposition techniques (wet chemistry, e-beam, rf sputtering); sample evaluation to include ellipsometry, photo-acoustic spectroscopy, adhesion testing, optical properties (spectral reflectivity and scattering), chemical properties of interface region (AES, SIMS, and ESCA) sample morphology (SEM and optical microscopy), x-ray diffraction, Raman spectroscopy.

219. SPUTTER-DEPOSITED COATINGS FOR OPTICAL APPLICATIONS — $125,000 — 02-2
W. T. Pawlewicz, P. M. Martin, D. D. Hays

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

PACIFIC NORTHWEST LABORATORY (continued)

220. NANOMETER MACHINING AND GRINDING DEVELOPMENT $90,000 02-5
D. M. Miller and N. Laegreid

Utilize unique Omega-X Machine Tool to develop machining technology permitting achievement of surface roughness less than 1.5 nanometer rms, and total contour accuracy of 100 nanometer for flat, concave, and convex spherical and aspherical surfaces up to one meter diameter. Identification and problem solving applied to machine tool, cutting tool, materials and part geometry limitations.

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221. STRESS CORROSION CRACKING AND ELECTROCHEMISTRY OF TRANSIENT CORROSION PROCESSES — $210,000 — 01-2

W. H. Smyrl
R. J. Salzbrenner

Crack propagation behavior of austenitic and ferritic stainless steels in molten $NaAlCl_4$ environments: anodic dissolution has been shown to be associated with crack extension. Selective dissolution of Cr from austenitic stainless steels occurs in the molten salt, and this was verified by Auger surface analysis. Further testing and electrodissolution measurements of austenitic steels are being pursued. Metallurgical variables will be investigated with high purity binary Fe alloys. Electrochemical and corrosion investigations are made with Digital Faradaic Impedance Measurements (DFIM).

222. ION IMPLANTATION AND DEFECTS IN MATERIALS — $600,000 — 01-3

P. S. Peercy
K. L. Brower
B. L. Doyle
H. J. Stein
D. M. Follstaedt
J. A. Knapp
S. M. Myers
S. T. Picraux

Modification and analysis of near surface regions of solids are being studied using ion beam techniques. Ion implantation metallurgy is used to determine phase diagrams, diffusion coefficients and solubilities, and to investigate the trapping of hydrogen and temper embrittling species in Fe and Ni. Ion implantation, ion beam mixing, laser and electron beam annealing are used to form equilibrium and nonequilibrium alloys which are then studied using ion beam analysis and electron microscopy techniques. Corrosion, diffusion, and electrical behavior are studied in amorphous metal surface layers, and in semiconductors formed by ion implantation. Ion beam techniques are used to control disorder and H in amorphous silicon to permit investigation of the fundamental structure and defect properties. Defects and metastable solutions in ion implanted and laser-annealed semiconductors are studied using EPR and optical techniques.

SANDIA NATIONAL LABORATORIES-Albuquerque (continued)

223. EROSION AND WEAR IN A FLUID ENVIRONMENT — $240,000 — 01-5

R. E. Cuthrell D. M. Mattox
E. Randich

Basic studies on the fracture, erosion and wear of surfaces in varying thermal and chemical environments. Effects of chemical environment on the fracture of brittle materials (chemomechanical effects) under well controlled environments using sensitive fracture detection techniques such as acoustic emission, exoelectron/exoion emission and photon emission. Failure analysis of fractured surfaces with modeling of the failure mechanisms. A study of the chemical vapor deposition conditions necessary to produce wear resistant coatings of refractory, hard borides and carbides. Gas-solid phase diagrams have been calculated and applied to the chemical vapor deposition of TiB_2, ZrB_2, TaB_2, and B_4C.

224. SEMICONDUCTORS FOR USE AT HIGH TEMPERATURES — $200,000 — 01-5

L. R. Dawson
I. J. Fritz
P. L. Gourley
G. C. Osbourn

Experimental and theoretical studies of bulk and interfacial high temperature properties of wide bandgap semiconductors ($Eg \geq 1.4$ eV). Objective is identification of candidate materials and contact metallizations suitable for high temperature (to 500°C) active semiconductor devices. The work has a comprehensive fundamental scope, incorporates modern materials growth techniques and is coordinated with device physics programs to give this research technological impact. Studies include doping, transport, optical and defect properties. Current emphasis has been on GaP and GaP-based materials.

225. SURFACE PHYSICS RESEARCH — $230,000 — 02-2

M. L. Knotek D. R. Jennison
J. E. Houston R. R. Rye
J. A. Panitz G. L. Kellogg

A broad range of experimental and theoretical studies are being conducted aimed at understanding the interaction of atoms and molecules with solid surfaces. The unique aspects of Auger Electron Spectroscopy are being exploited to study the variation of electronic properties during such interactions. The local chemical environment of surface and adsorbes species is obtained using gas-phase molecules as "absolute" standards along with theoretical analyses of the spectroscopic results. The imaging and mass spectroscopic abilities of the field-ion and field-desorption techniques are being developed to study the morphology of biological and other molecules, and the Pulsed Laser Atom Probe is being applied to studies of adsorption and reaction intermediate states of molecules interacting with the various planes of well defined transition metal surfaces.

SANDIA NATIONAL LABORATORIES-Albuquerque (continued)

226. DEVELOPMENT OF A FIELD-DESORPTION MICROSCOPE FOR SURFACE IMAGING — $30,000 — 02-5
J. A. Panitz

A point projection microscope has been developed which utilizes field desorption techniques to obtain images of the morphology of biomolecular adsorbates on a cryogenically cooled emitter tip. This apparatus will include the capability of time-of-flight mass analysis of desorbed species, automated dosing of biomolecular species with the blanket gas, and the ability to digitally store and process image data. Both positive and negative images of ferritin have recently been obtained with an estimated resolution of better than three nanometers. Preliminary images of hemocyanine have also been obtained.

227. SOLAR PHOTOASSISTED ELECTROCHEMICAL CELLS: DEVELOPMENT OF NEW MATERIALS FOR HYDROGEN AND OTHER CHEMICAL PRODUCTION — $100,000 — 02-2
D. S. Ginley, R. C. Hughes, M. A. Butler, A. K. Hayes, D. M. Haaland, G. W. Arnold

The basic charge transfer mechanisms involved in photocatalytic and photosynthetic reactions of semiconductor/electrolyte interfaces are being investigated with special attention directed to an understanding of stability and stabilizing techniques. Studies of the interfacial region directed at improving photoelectrochemical cell performance include: surface modification to improve catalytic behavior, overcoating with corrosion resistant materials, and new materials development. New instrumental methods are being developed to directly probe the solid/electrolyte interface. Some of these techniques are sub-band-gap photocurrent spectroscopy, Fourier transform infrared spectroscopy, ion scattering techniques, electrochemical ion implantation and photoemission spectroscopy. A laser scanning system is being constructed to allow depth resolved photoresponse maps of electrode surfaces.

228. STUDIES OF THE VAPOR PHASE OF THE CHEMICAL-VAPOR-DEPOSITION PROCESS — $175,000 — 02-2
A. W. Johnson, W. G. Breiland, P. J. Hargis, M. E. Coltrin

Studies of important vapor-phase reactions and nucleation processes during CVD deposition of photovoltaic cells and corrosion-resistant coatings, measurements of major and minor species densities, gas temperatures, fluid flows, and gas-phase particulate distributions using laser Raman and Mie scattering and laser induced fluorescence. Development of a predictive model including chemical kinetics and fluid dynamics. Consideration of the applications of laser-assisted CVD.

SANDIA NATIONAL LABORATORIES-Albuquerque (continued)

229. ELECTRON AND PHOTON-STIMULATED DESORPTION $175,000 02-2

M. L. Knotek G. M. Loubriel

Studies of metal, metal oxide, semiconductor and alkali halide surfaces as well as their interactions with H_2O, H_2, O_2 and other adsorbates are being carried out using Electron- and Photon-stimulated desorption techniques (ESD and PSD). These investigations exploit the discovery that desorption occurs by Auger decay of radiation induced core holes. This allows the extraction of site specific, adsorbate specific electronic and structural information since both local empty density of states and extended x-ray absorption fine structures are sampled. These techniques are uniquely surface sensitive and sample only the uppermost layer of surface atoms. The high sensitivity to hydrogen will be exploited in the study of its role in catalysis, corrosion and semiconductor technology.

SANDIA LABORATORIES
Livermore, California 94550

Walter Bauer - Phone (FTS) 532-2994 or (415) 422-2994

230. PROTECTIVE BARRIERS AND COATINGS FOR COMBUSTION MATERIALS — $200,000 — 01-1

P. L. Mattern (FTS) 532-2520 (Comm) (415) 422-2520
R. E. Benner
A. S. Nagelberg
J. C. Hamilton

A long-term, materials-oriented program to study corrosive/erosive processes at high temperatures. A Materials Research Combustion Simulator, a facility for simulating relevant combustion environments, will be developed and installed at the Combustion Research Facility at Sandia National Laboratories in Livermore. Initial emphasis will be given to the study of molten salt corrosion and gas phase oxidation in materials and coatings for use in advanced turbines. Optical diagnostic methods will be used to characterize the simulated environments, and to monitor surface processes during exposure. Post-exposure analysis techniques will be developed and implemented where appropriate.

231. GASES IN METALS — $200,000 — 01-2

W. D. Wilson
G. J. Thomas
M. I. Baskes
R. J. Bastasz

This is a coupled experimental and theoretical program aimed at understanding the behavior of helium and hydrogen in metals and their influence on mechanical properties. Quantum theoretical calculations show that small clusters of helium atoms produce embryonic helium bubbles and associated self-interstitials in the absence of radiation damage. Sub-threshold helium implantations at low temperatures show the existence of these bubbles using transmission electron microscopy. Tritium experiments utilize the decay of tritium into helium for damage-free injection and also for autoradiographic measurements via detection of the beta particles. Measurements of diffusion and trapping have been performed.

232. DIAGNOSTICS FOR COMBUSTION MATERIALS RESEARCH — $100,000 — 02-5

P. L. Mattern (FTS) 532-2520 (Comm) (415) 422-2520
R. E. Benner
R. L. Farrow
J. C. F. Wang

A long-term, materials-oriented program to study corrosive/erosive processes at high temperatures. A Materials Research Combustion Simulator, a facility for simulating relevant combustion environments, will be developed and installed at the Combustion Research Facility at Sandia National Laboratories in Livermore. Initial emphasis will be given to the study of molten salt corrosion and gas phase oxidation in materials and coatings for use in advanced turbines. Optical diagnostic methods will be used to characterize the simulated environments, and to monitor surface processes during exposure. Post-exposure analysis techniques will be developed and implemented where appropriate.

SOLAR ENERGY RESEARCH INSTITUTE
1617 Cole Boulevard
Golden, Colorado 80401

General Research Division - Materials Research Branch
B. L. Butler - Phone: (FTS) 327-1104 or (303)231-1104

233. SOLAR MATERIALS RESEARCH $280,000 01-1
A. W. Czanderna, P. Schissel, J. Webb,
R. Pitts, T. Thomas

Mechanisms of materials degradation affecting the performance in solar energy conversion systems; interface studies in the glass/silver, silica/silver, silver/copper and silver/polymer systems; silver deposition by evaporation, sputtering, and electroless deposition; polycrystalline silver films characterized for reflectance, topography, structure, composition, and adhesion; stability of polymer/silver interfaces, with emphasis on polycarbonate and polymethymethacrylate; degradation in simulated solar environments; UV radiation, environmental oxidizing and sulfur bearing gases, and atmospheric pressures; interfacial catalytic and corrosion effects; diffusion; SEM, EDX, XPS, SIMS, ISS, SAM, and FT-IR.

Gordon Groves - 327-1228
1129

Stan Bull - X7723

SECTION B

Contract Research

(Primarily Universities)

This information was prepared by the DOE project monitor. There is considerable (about 10%) turnover in the Contract Research program and some of the projects will not be continued beyond the current contract period.

AMERICAN INSTITUTE OF PHYSICS

301. A HISTORY OF SOLID STATE PHYSICS — $ 53,692 (3 years) — 02-2

S. R. Weart - Center for History of Physics
Phone: (212)-661-9404
L. Hoddeson - Department of Physics, University of Illinois
Phone: (217)-333-4779

Participation in an international project to produce a written history of modern solid state science. AIP will concentrate on North American research. Will include oral history interviews. Encourage organizations and individuals to preserve archival papers and documents.

ARIZONA STATE UNIVERSITY

302. IMAGING SURFACES AND DEFECTS IN CRYSTALS — $ 80,180 — 02-2

J. M. Cowley - Dept. of Physics
Phone: (602)-965-6459

High resolution scanning transmission electron microscope study of surface reaction products by electron microdiffraction and selective imaging. In particular, a study of the crystal structure, morphology and epitaxial relationships of oxide microcrystals formed on chromium thin films and iron-chromium alloys. Also, parallel studies on the oxidation of bulk crystals by the methods of reflection electron diffraction, scanning electron microscopy and dark-field scanning microscopy on pyrolytic graphite.

BATTELLE COLUMBUS LABORATORIES

303. FAILURE OF CERAMICS FROM MULTIAXIAL STRESSES — $136,290 — 01-5

A. R. Rosenfield, D. K. Shetty, S. G. Sampath, W. H. Duckworth
Phone: (614)-424-4353

Understanding of multiaxial stress phenomena on the mechanical behavior of ceramics. Relationship of stress-state effects to stress-intensity factor. Effects of tensile and shear stresses parallel to an artificial crack and effects of stress ratios on strength in ceramic specimens containing natural flaws to evaluate statistical (Weibull) descriptions of strength. Materials preparation and characterization. Fractography. Three dimensional linear elastic finite element analysis of test-specimen geometries and for stress-intensity factors. Biaxial tests of ceramic specimens containing controlled artificial flaws.

BOSTON UNIVERSITY

304. INFRARED ABSORPTION SPECTRUM OF FREE CARRIERS IN POLAR SEMICONDUCTORS — $ 51,700 — 02-3

B. Jensen - Dept. of Physics
Phone: (617)-353-2610

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

BROWN UNIVERSITY

305. A COMBINED MACROSCOPIC AND MICROSCOPIC APPROACH TO THE FRACTURE OF METALS — $176,000 — 01-2

R. J. Asaro - Division of Engineering
Phone: (401)-863-2317
J. Gurland - Division of Engineering
Phone: (401)-863-2628
A. Needleman - Division of Engineering
Phone: (401)-863-2863

Analysis and measurement of fracture in metals, principally steels; stable crack growth in elastic-ideally plastic materials under small scale yielding conditions and application of model to high strength steels; cavitation as a function of plastic strain, particle size, stress triaxiality, and H_2 activity during ductile fracture of plain carbon steels; creep cavity growth in deformation vs diffusion controlled fields; validity of singularities describing crack tip strain fields during load transients.

306. TIME RESOLVED FAR INFRARED SPECTROSCOPY OF EXCITONS — $ 62,000 — 02-2

A. V. Nurmikko - Division of Engineering
Phone: (401)-863-2869
M. Glicksman - Division of Engineering
Phone: (401)-863-2869

High-resolution, time-resolved spectroscopy of excitons in semiconductors at far IR wavelengths with subnanosecond speed. Will use tunable submillimeter wave laser to study III-V and II-VI semiconductors.

CALIFORNIA INSTITUTE OF TECHNOLOGY

307. MELTING IN ADSORBED FILMS — $ 79,462 — 02-2

D. Goodstein - Dept. of Physics and Applied Physics
Phone: (213)-795-6811

Study of two-dimensional melting of methane on Grafoil. Systematic thermodynamic measurements will be made in the temperature range 2-100K with coverages of 0-5 monolayers. Dynamic studies will be made using pulsed NMR.

308. STUDIES OF ALLOY STRUCTURE AND PROPERTIES — $185,000 — 01-1

William L. Johnson - Division of Engineering and Applied Science
Phone: (213)-356-4433

Synthesis, structure and properties of amorphous alloys; electronic structure and superconductivity; flux pinning by crystalline precipitates; low temperature calorimetry; magnetic impurities and ordering in superconductors; local chemical and physical structure using AXD, EXAFS, X-ray Raman scattering and Mössbauer techniques; measurements of creep, ductility, yield strength and tensile strength; effects of irradiation on superconducting and mechanical properties; "point defect" structure in amorphous materials using X-ray diffraction, Mössbauer spectroscopy, internal friction and position annihilation spectroscopy.

309. THE PRESSURE DEPENDENCE OF THE MECHANICAL PROPERTIES OF POLYMERS — $ 58,000 — 01-2

N. W. Tschoegl - Dept. of Chemistry and Chemical Engineering
Phone: (213)-356-4676

Development of constitutive equations describing time-temperature-pressure effects on creep relaxation in elastomers; determination of compressibility and thermal expansion up to 10 kbars; time-dependent Poisson ratio measurement; analysis of behavior near glass transition temperature.

UNIVERSITY OF CALIFORNIA/DAVIS

310. RADIATION DAMAGE AND ENVIRONMENTAL EFFECTS IN NUCLEAR WASTE STORAGE MEDIA — $ 72,000 — 01-1

D. G. Howitt - Dept. of Mechanical Engineering
Phone: (916)-752-1164, 0580

Comparative evaluation of the response of nuclear waste storage glasses and candidate crystalline ceramics to irradiation is being studied over a range of temperatures in a variety of irradiation environments to determine the microstructural features enhancing deterioration and radiation instability in these materials. Effects of microstructural features, phase separation, precipitation, devitrification, particle size, and composite annealing temperatures on the properties of nuclear waste storage media. Numerical calculations of non-linear composition profiles in leached waste storage media.

311. DEFORMATION MECHANISMS AND FAILURE MODES IN SUPERPLASTICITY — $ 72,748 (14 months) — 01-2

A. K. Mukherjee - Dept. of Mechanical Engineering
Phone: (916)-752-1776

Experimental and analytical study of superplastic deformation of metals, specifically Zn-Al, Ni-base, and Cu-base alloys; measurement of creep as a function of stress, temperature, strain rate, and microstructure, e.g., grain size, identification of controlling intragranular and intergranular as well as independent and parallel creep mechanisms in alloys after various thermomechanical processing; relationship of above to superplastic forming.

312. AN INVESTIGATION OF THE ROLE OF SINTERING IN GAS-SOLID INTERACTIONS — $ 72,000 — 01-3

Z. A. Munir - Dept. of Mechanical Engineering
Phone: (916)-752-0559, 0580

Investigation of the role of sintering in the kinetics of gas-solid interactions in powder compacts. Influence of surface transport and bulk transport sintering on the kinetics of dissociation reactions of the type $CaCO_3(s) \rightleftharpoons CaO(s) + CO_2(g)$, and of reduction reactions of the type $FeO(s) + H_2(g) \rightleftharpoons Fe(s) + H_2O(g)$. Morphological changes (surface area, pore size, and overall porosity) will be measured and related to changes in the rates and reversibility of interactions of the types indicated above.

UNIVERSITY OF CALIFORNIA/IRVINE

313. RAMAN SPECTROSCOPY OF MOLECULAR ADSORBATES — $105,000 — 02-2

J. C. Hemminger - Dept. of Chemistry
Phone: (714)-833-6020
S. Ushioda - Dept. of Physics
Phone: (714)-833-6619

Combine Raman spectroscopy and modern surface science technology to study binding and chemistry of adsorbates on well characterized surfaces. Study mechanism of "giant" enhanced Raman scattering. Correlate enhancement with surface roughness on stepped and kinked surface of Ag. Also correlate enhancement with electronic energy levels of metal-adsorbate system as determined by electron energy loss spectroscopy. Apply Raman spectroscopy to study of corrosion by H_2S and O_2.

314. INTERACTION OF LOW ENERGY ELECTRONS WITH SURFACE LATTICE VIBRATIONS — $ 85,800 — 02-2

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

Theory of inelastic scattering of electrons by vibrating atoms and molecules at solid surfaces. Role of image potential in electron energy-loss spectroscopy (EELS) with low impact energies. Applications to H on W, and NH_3 and CO on Ni, Pt, Rh, and Ir. Theory of lattice dynamics of clean and adsorbate-covered surfaces and of thermal diffuse scattering of electrons from clean transition metal surfaces. This program is strongly coupled with that of S. Y. Tong, University of Wisconsin - Milwaukee.

UNIVERSITY OF CALIFORNIA/LOS ANGELES

315. IRRADIATION-INDUCED PRECIPITATION AND SOLUTE SEGREGATION IN ALLOYS — $ 92,805 — 01-4

A. J. Ardell - Materials Department
Phone: (213)-825-2942

Irradiation-induced solute segregation and precipitation in Pd and Ni-base alloys; 20-750^{o}C; proton, electron and heavy-ion irradiations to 0.25 dpa; effects of dose, dose rate, temperature, solute size misfit, damaging particle and alloy composition; voids; irradiation effects in metallic glasses; TEM, analytical electron microscopy and HVEM.

UNIVERSITY OF CALIFORNIA/SAN DIEGO

316. THE RESPONSE OF SUPERCONDUCTING TO VARIATIONS IN IMPURITY CONTENT AND APPLIED PRESSURE — $219,919 — 02-2

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

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

317. RESEARCH ON THE THERMOPHYSICAL PROPERTIES OF MATERIALS — $115,484 — 02-5

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

Studies of the science of heat engines and the materials which work in them. The following specific areas are included: (1) Heat engines (Stirling-Malone and Brayton cycles) using liquid working substance and their possible application to the heating and cooling of structures, (2) Basic thermal and mechanical principles of a prime mover (Stirling-Malone cycle) using liquid water as working substance, (3) Fundamental reexamination of heat engine science using cryogenic temperatures and the helium isotopes as working substances, (4) Gravitational convection of energy in dilute solutions of ^3He in superfluid ^4He as a model of convective processes in a low Prandtl number insulating fluid where stochastic processes are known to be important, (5) Search for a quasi-particle-driven instability in ^3He-^4He solutions near the tricritical point, (6) Preliminary experimental considerations on the study at low temperatures of both the "electron in vacuum" and the "electron bubble in superfluid ^4He" non-neutral plasmas.

UNIVERSITY OF CALIFORNIA/SANTA BARBARA

318. RESONANCE STUDIES OF SUPERIONIC CONDUCTORS — $154,019 (2 years) — 02-2

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

NMR and EPR study of superionic and related compounds. Computer simulation of ion hopping processes. Low frequency measurements on $Mn:PbF_2$. $H:CaF_2$ and $HiPbF_2$ to determine importance of H^- diffusion and its relation to F^- mobility in ionic conduction. Determine charge states of Fe in $Co^{57}:PbF_2$ by Mössbauer studies.

*Also at Los Alamos National Laboratory

CARNEGIE INSTITUTE OF WASHINGTON

319. STUDY OF THE PROPERTIES OF HYDROGEN AT STATIC PRESSURES OF ONE MEGABAR — $138,250 (19 months) — 02-2

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

Investigations of hydrogen under very high pressure. Hydrogen was pressurized to 900 Kbar, and a static pressure of 650 Kbar was achieved. Laser Raman scattering of molecular bonding phenomena as a function of pressure in hydrogen and deuterium. Brillouin scattering measurements of hydrogen up to 250 Kbar. Single crystals of neon examined up to 250 Kbar. X-ray pressure cell development.

CARNEGIE-MELLON UNIVERSITY

320. RESEARCH ON PHASE TRANSFORMATIONS AND NON-EQUILIBRIUM PROCESSES — $ 69,430 — 02-3

J. S. Langer - Dept. of Physics
Phone: (412)-578-2762

Theory of certain non-equilibrium processes of importance in design of metallurgical materials. Theory of dendritic crystal growth. Theory of eutectic solidification with emphasis on roles played by fluctuations and instabilities. Numerical and analytic studies of theory of interfacial morphology. Kinetics of phase separation in alloy solids and multi-component fluids.

321. FUNDAMENTAL STUDIES OF EROSION AND EROSION/CORROSION FOR COAL GASIFICATION SYSTEMS — $ 53,000 — 01-5

J. C. Williams - Dept. of Metallurgy and Materials Science
Phone: (412)-578-2704
G. B. Sinclair - Dept. of Mechanical Engineering
Phone: (412)-578-2504

Particulate erosion of ductile metals investigated for conditions of normal impact of rigid spherical particles; strain distribution obtained based on the elastic plastic behavior of metals at high strain rates; multiple impacts treated as quasi-fatigue cycles, leading to erosion loss described by a Coffin-Manson-type relationship; experiments with single and multiple particle impacts to measure substrate displacement, weight loss, and microstructural features such as crack paths and substructural changes; materials - Cu, Cu-Al alloys, steels; techniques - laser interferometry, electron microscopy, finite element analysis.

CASE WESTERN RESERVE UNIVERSITY

322. COUPLED DIFFUSION PHENOMENA IN MULTICOMPONENT GLASSES AND GLASS FORMING LIQUIDS — $ 85,000 — 01-3

A. R. Cooper - Dept. of Metallurgy and Materials Science
Phone: (216)-368-4224

Study of rate processes, e.g., precipitation, dissolution and phase separation in multicomponent systems at high temperatures. Study of transport processes and thermodynamics in multicomponent molten silicate systems, and kinetics of these processes in such systems. Relation of the interdiffusion coefficient matrix to the individual ionic species mobilities or self-diffusion coefficients. Work focused on systems K_2O-SrO-SiO_2 and CaO-Al_2O_3 SiO_2. Ultimate goal is a sufficiently well-documented understanding of such transport processes that will be useful for prediction of behavior in the many high temperature processes that involve molten silicates.

323. ENVIRONMENT REACTIONS AND THEIR EFFECTS ON MECHANICAL BEHAVIOR OF METALLIC MATERIALS — $ 91,700 (18 months) — 01-2

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

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

324. MICROSTRUCTURAL DEVELOPMENT IN OXIDE CERAMICS — $ 90,000 — 01-2

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

Effect of non-stoichiometry on plastic deformation in UO_{2+x}. Mechanism and kinetics of formation of crystallographic shear planes in reduced rutile, TiO_{2-x}. Evaluation and stability of microstructure in fusion-cast MgO-$MgAl_2O_4$ refractories used for MHD heat exchangers.

CASE WESTERN RESERVE UNIVERSITY (continued)

325. EXPERIMENTS IN HIGH VOLTAGE AND ANALYTICAL ELECTRON MICROSCOPY — $123,000 — 01-4

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

Irradiation damage study in metals and ceramics by high voltage electron microscopy with supplementary experiments using ions and neutrons for comparison purposes. Irradiation effects in alloys include defect clustering, phase stability, precipitate growth and order/disorder phenomena, particularly in ordered fcc structures (Ni_3Al) and ordered bcc structures (NiAl). Irradiation effects in ceramics include amorphization by ionization damage in SiO_2 and GeO_2 polymorphs and various silicates, displacement damage leading to the formation of defect clusters in simple oxides such as MgO, NiO and BeO, void growth in oxides susceptible to swelling such as Al_2O_3, and phase decomposition and defect stabilization in more complex swelling-resistant ceramics such as spinels and nitrides.

CATHOLIC UNIVERSITY OF AMERICA

326. IONIC TRANSPORT AND ELECTRICAL RELAXATION IN GLASS — $ 56,690 — 01-3

C. T. Moynihan - Vitreous State Laboratory
Phone: (202)-635-5328

Ionic transport in glass. Analysis and modelling of electrical transport data coupled with dielectric relaxation measurements covering a wide frequency and temperature range. Theory of mixed alkali effect in glass and application of Debye-Falkenhagen theory to dielectric relaxation in low alkali glasses. Characterization of hydrated surface layer formation using complex impedance measurements and of high frequency dielectric losses in glass. Dielectric relaxation effects on order parameter theory for structural relaxation in glass. Computer modelling of thermally stimulated depolarization currents (TSDPC) for ionically conducting glasses using as input dielectric relaxation data obtained in the frequency domain.

UNIVERSITY OF CHICAGO

327. RESEARCH IN THE THEORY OF ELEMENTARY PARTICLES AND CONDENSED MATTER — $115,721 — 02-3

L. P. Kadanoff - James Franck Institute
Phone: (312)-753-8205
Y. Nambu - Enrico Fermi Institute
Phone: (312)-753-8608

The research aims to elucidate problems which are relevant to both elementary particle physics, through quantum field theory, and condensed matter physics--via the statistical mechanics of phase transitions. String theories and problems in two-dimensions of space (or one of space and one of time) will get considerable attention. Topics under consideration will include Hamiltonian and equation of motion methods for approaching string theory, multicritical points and bifurcation theory in two dimensions, parafermion fields, Monte Carlo renormalization group analyses, and studies of the stability of gauge theories under small perturbations.

COLORADO SCHOOL OF MINES

328. FERROUS ALLOY METALLURGY - LIQUID LITHIUM CORROSION AND WELDING — $135,000 — 01-5

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

Embrittling effect of liquid lithium on ferrous alloys; influence of welding parameters on the microstructure and mechanical properties of dissimilar ferrous metal weldments; effect of liquid lithium on the fatigue behavior of 2¼ Cr-1 Mo steel; Auger electron spectroscopy of fracture surfaces; role of microchemistry and structure on weld mechanical properties; dissimilar welds in 2¼ Cr-1 Mo/316 stainless steel; gas metal arc weld strip overlay cladding process.

COLUMBIA UNIVERSITY

329. DEFECT INTERACTIONS AT HIGH CONCENTRATIONS IN SOLID OXIDE ELECTROLYTES — $ 55,997 — 01-3

A. S. Nowick - Krumb School of Mines
Phone: (212)-280-2921

Interactions of defects at high concentrations in oxides that are fast-ion conductors; CeO_2 doped with Y and Sc; study of relationship between defect structure and electrical properties; relationship between simple defects that form at low concentrations and the ordering and microdomain formation observed at high concentrations; kinetics of cationic ordering. Electrode phenomena. Complex impedance plots and the "grain-boundary effect." Anelastic relaxation. Neutron scattering. Ionic thermo-current dielectric relaxation defect studies. Synchrotron EXAFS experiments.

UNIVERSITY OF CONNECTICUT

330. ELECTRODE POLARIZATION STUDIES IN HOT CORROSION SYSTEMS — $ 64,500 — 01-3

O. F. Devereux - Dept. of Metallurgy
Phone: (203)-486-4714

Electrode polarization behavior of Ni in molten salts based on either Na_2CO_3 or FeS + Na_2S; anodic and cathodic half cell reactions identified at various O:S activities in the electrolyte; kinetics and mechanisms of corrosion established; sulfidation of Fe measured in gaseous environments.

331. ELECTRON-DISLOCATION INTERACTIONS AT LOW TEMPERATURES — $ 55,397 — 01-2

J. M. Galligan - Dept. of Metallurgy
Phone: (203)-486-3541, 4623

Determination, in an ordinary tensile test, of velocity of mobile dislocations, electron-dislocation drag, and mobile dislocation density. Experiments measure change in stress for plastic deformation accompanying change in magnetic field. Effects of crystal orientation. Occurrence of magneto-oscillations in stress field as a function of temperature, magnetic field, and applied strain rate at specific angles relative to principal axes of a crystal.

UNIVERSITY OF CONNECTICUT (continued)

332. INVESTIGATION OF ROLE OF SUBSURFACE ZONES IN WEAR OF MATERIALS — $ 75,000 — 01-5
S. Rice - Dept. of Mechanical Engineering
Phone: (203)-486-2153

Experimental characterization of the formation, composition and morphology of subsurface zones and wear debris for material pairs making solid contact both in sliding and impact modes; experimental investigation of the roles of nominal contact stress, relative sliding velocity and effective contact stiffness of subsurface zone formation, composition and morphology; analytical prediction of the equilibrium configuration of subsurface morphology for a work hardening elastoplastic material subject to given load cycling and temperature distributions; model development which allows prediction of composition and morphology of subsurface zones for selected materials subjected to both sliding and impulsive contact; and postulation and experimental investigation of in situ development of wear resistance.

CORNELL UNIVERSITY

333. INFLUENCE OF GRAIN BOUNDARIES ON THE ELECTRICAL TRANSPORT PROPERTIES OF POLYCRYSTALLINE SI FILMS — $ 70,700 — 01-1
D. G. Ast - Dept. of Materials Science and Engineering
Phone: (607)-256-4140

Characterization of the structure and electrical activity of defects in hot pressed Si and in single crystals grown by the EFG process; examination of Shockley partial dislocations and second order twins at coherent twin boundaries; comparison of deformation-induced vs as-grown dislocation activity; passivation of grain boundaries with hydrogenation and thermal treatments; techniques used: HVEM, TEM, electron beam induced charge in SEM.

334. INITIAL STAGES OF OXIDATION OF METALS — $ 98,500 — 01-1
J. M. Blakely - Dept. of Materials Science and Engineering
Phone: (607)-256-5149

Investigation of the initial stages of oxidation of metals--kinetics, oxide composition and structure, and transition from thin to thick films; sequential formation of Fe_3O_4, FeO, and NiO during oxidation of $Fe_{40}Ni_{60}$; evolution of BeO on (0001) Be; techniques used: LEED, AES, TEM, and (planned) synchrotron.

CORNELL UNIVERSITY (continued)

335. ENVIRONMENT AND FRACTURE — $ 87,000 — 01-2

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

Experimental investigation of H_2 permeation through metals, primarily steels; chemical and physical trapping, trapping sites, densities, and characteristic binding energies for dislocations and substitutional solute atoms; influence of prior cold work and applied stress level on H_2 trapping, solubility, and diffusivity; effects of macroscopic trap distribution, e.g., uniform vs gradients near surfaces, and of surface coatings on H_2 permeation; modelling of H_2-attack of steels and the resulting Nelson curves in terms of physical parameters such as methane fugacity, bubble density, etc.

336. INELASTIC DEFORMATION IN NON-METALLIC CRYSTALLINE SOLIDS — $ 47,500 (11 months) — 01-2

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

Liquid-phase hot-pressing and high-temperature deformation of hot-pressed TiC and TiC-VC, and the effects of excess Ti and TiB_2 precipitates on such materials. Densification mechanisms and kinetics. Creep and constant compressive strain rate experiments. TEM-STEM analysis.

337. MECHANICAL PROPERTIES OF CRYSTALLINE SOLIDS — $145,000 — 01-2

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

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

CORNELL UNIVERSITY (continued)

338. PROBABILISTIC MODELS OF THE STRESS-RUPTURE OF COMPOSITE MATERIALS — $ 77,800 — 01-2

S. L. Phoenix - Sibley School of Mechanical & Aerospace Engineering
Phone: (607)-256-3462

Modelling tensile and stress rupture strengths of fiber reinforced polymer composites based on a probabilistic distribution of fiber strengths; development of asymtotic analyses and application of these to the tensile strength of composites with different shapes and load sharing rules; effect of matrix viscoelasticity on creep and stress rupture for carbon, S-glass, and Kevlar fibers in polyester and epoxy matrices; influence of fiber strength variation (Weibull modulus) on the importance of matrix properties.

339. HIGH TEMPERATURE MECHANICAL BEHAVIOR OF SILICON NITRIDE — $ 74,000 — 01-2

R. Raj - Dept. of Materials Science and Engineering
Phone: (607)-256-4040

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

340. DIFFRACTION AND MICROSCOPY STUDIES OF THE STRUCTURE OF GRAIN BOUNDARIES IN Fe, Fe-BASE ALLOYS, AND CERAMIC MATERIALS — $109,900 — 01-1

S. L. Sass, Dept. of Materials Science and Engineering
Phone: (607)-256-5239

Investigation of grain boundary structure in metals and ceramics, primarily Fe-base alloys, Al_2O_3 and NiO; characterization of boundary periodicity, unit cell, and dislocation arrays, using direct imaging in TEM and electron and X-ray diffraction.

CORNELL UNIVERSITY (continued)

341. DEFECTS IN METAL CRYSTALS — $355,000 (2 years) — 01-4
David M. Seidman - Dept. of Materials Science and Engineering
Phone: (607)-256-2365

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

DARTMOUTH COLLEGE

342. THE ROLE OF GRAIN SIZE ON THE BRITTLE TO DUCTILE TRANSITION OF THE STRONGLY ORDERED ALLOY Ni_3Al — $ 57,200 — 01-2
E. M. Schulson - Thayer School of Engineering
Phone: (603)-646-2888

Characterization of Ni_3Al powder produced by rapid solidification; consolidation by extrusion; measurement and correlation of grain size with mechanical behavior; use of SEM to evaluate fracture morphology and AES to examine impurity segregation to grain boundaries.

343. SUPERCONDUCTIVITY IN FILAMENTARY EUTECTIC COMPOSITES — $109,000 (2 years) — 02-2
M. P. Zaitlin - Dept. of Physics and Astronomy
Phone: (603)-646-3270

Samples containing niobium filaments in a thorium matrix offer surprising challenges to the understanding of superconducting materials. Measurement of the thermal and electrical conductivity made near the superconducting transition temperature should show coupling between the filaments and between the filaments and the matrix. This coupling is expected to produce a crossover from one-dimensional to three-dimensional superconductivity. Such parameters as filament size, filament spacing as well as matrix composition offer variability in addition to the usual superconductivity measurements.

UNIVERSITY OF DELAWARE

344. ANALYSES OF FAILURE MODES IN SHORT FIBER REINFORCED THERMOPLASTICS — $ 42,100 — 01-2

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

Calculation of physical and mechanical properties of polymers reinforced with discontinuous fibers; thermoelastic constants, thermal conductivity, and elastic and shear moduli found for the unidirectional (parallel) fiber case using variational and statistical methods.

345. RADIATION EFFECTS IN AMORPHOUS METALLIC ALLOYS — $ 69,510 — 02-2

R. B. Murray - Dept. of Physics
Phone: (302)-738-2147
D. G. Onn - Dept. of Physics
Phone: (302)-738-2661
J. J. Kramer - Dept. of Electrical Engineering
Phone: (302)-738-8170

The effects of irradiation on the magnetic and electrical properties of amorphous ferromagnetic alloys of Fe-Ni-P-B will be studied. Small angle x-ray scattering, Auger, transmission electron microscopy, and Kerr magneto-optic dynamical domain studies will be used to delineate the mechanism(s) leading to these changes.

UNIVERSITY OF DENVER

346. THE DETECTION OF HYDROGEN ASSISTED CRACK GROWTH — $ 74,100 (15 months) — 01-5

S. H. Carpenter - Dept. of Physics
Phone: (303)-753-2238

Experimental investigation of H_2 induced deformation and cracking in steels; measurement of kinetics of cracking during exposure to H_2 with and without applied stress; influence of vacuum annealing on crack healing; techniques used -- acoustic emission, modulus defect.

UNIVERSITY OF DENVER (continued)

347. THERMAL EXPANSION EFFECTS IN CORDIERITE — $ 73,000 — 01-3

P. K. Predecki - Dept. of Chemistry
Phone: (303)-753-2141

Effect of solid solutions of various sized ions in cordierite on thermal expansion. Solutes considered are Ge, B, and P substituted on tetrahedral sites, Fe, Zn, Mn, Li, and Cr substituted on octahedral sites, and alkali and alkaline earth ions interstitially in the large c-axis channels. Measurement of lattice thermal expansion coefficient on powder samples over the range from 25° to 800°C by X-ray diffraction using a Huber-Guinier camera. Correlation of lattice thermal expansion with both lattice distortion and changes with X-ray diffracted intensity. Ultimate objective is to understand how changes in substitutional and interstitial lattice site occupancy and associated local bond distortions affect the lattice expansion coefficients.

DREXEL UNIVERSITY

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

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

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

EMORY UNIVERSITY

349. FAR INFRARED STUDIES OF SUPER-CONDUCTING V_3Si, Nb_3Ge and Nb — $ 85,660 — 02-2

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

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

FLORIDA STATE UNIVERSITY

350. POLYMERS IN MECHANO-CHEMICAL SYSTEMS: STRUCTURE-PROPERTY REQUIREMENTS — $ 55,000 — 03-1

L. Mandelkern - Dept. of Chemistry
Phone: (904)-644-2054

Studies of energy effects occurring in the crystal-liquid transition of oriented macromolecular systems. Equilibrium melting temperature-stress relations; kinetics of crystallization and melting under stress; a description of the morphological forms that result, and their influence on mechanical properties. Optimization of the functioning of mechano-chemical systems of polymers.

Hench — X 1457

UNIVERSITY OF FLORIDA

351. METAL DISSOLUTION KINETICS IN ORGANIC SOLVENTS USING ROTATING RING-DISC VOLTAMMETRY — $ 90,000 (15 months) — 01-3

J. R. Ambrose - Dept. of Materials Science and Engineering
Phone: (904)-392-1456

Characterization of electrochemistry of Ni-base binary alloys in alcohol solutions and Fe-base binary alloys in aqueous solutions; measurement of metal dissolution kinetics using rotating ring-disc voltammetry; identification of dominant processes and film formation.

352. SYNTHESIS AND CHARACTERIZATION OF NOVEL POLYMERS FROM NON-PETROLEUM SOURCES — $110,000 — 03-3

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

Synthesis and structural characterization of polysaccharide-based polymers for use in tertiary oil recovery with the following objectives: 1) preparation of very high intrinsic viscosity starch graft copolymers and the characterization of their structures, 2) correlation of intrinsic viscosity of these polymers with the number of grafts per starch molecule and degree of polymerization of the grafts, 3) synthesis of high intrinsic viscosity graft copolymers with a substantial polysaccharide (starch) content, and 4) preparation of polymeric materials of high intrinsic viscosity by chain extension of polysaccharides or polysaccharide graft copolymers. Experimental and theoretical studies of the dependence of shear degradation of copolymers on their molecular structures.

GENERAL ELECTRIC CORPORATE RESEARCH AND DEVELOPMENT

353. A STUDY OF SOLID STATE METAL/CERAMIC REACTIONS — $ 69,930 — 01-5

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

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

354. LOCAL ATOMIC AND ELECTRONIC STRUCTURE IN GLASSY METALLIC ALLOYS — $ 95,504 — 02-2

R. P Messmer - Materials Characterization Laboratory
Phone: (518)-385-8488
J. Wong - Materials Characterization Laboratory
Phone: (518)-385-8463

Experimental and theoretical studies of amorphous iron, nickel, boron and phosphorous metallic glasses. Extended x-ray absorption fine structure (EXAFS) measurements using synchrotron radiation will be used to characterize the local environment of the metal atoms. Quantum mechanical calculations for small model systems will be used to establish the fundamental nature of the interactions between the constituent elements in the alloy to include the specificity of Fe-P, Ni-B interactions as well as metalloid-metalloid interactions.

GEORGIA INSTITUTE OF TECHNOLOGY

355. THE STRUCTURE AND REACTIVITY OF HETEROGENEOUS SURFACES AND STUDY OF THE GEOMETRY OF SURFACE COMPLEXES — $115,570 — 02-3

U. Landman - School of Physics
Phone: (404)-894-3368

The objective of the project is to provide a coherent, fundamental understanding of surface material parameters which control its structure, electronic and vibronic characteristics and reactivity. The studies involve analytical and computer simulation methods. Various properties which influence transport, diffusion, reactivity, structure reconstruction, vibrational and electronic spectra, stability and phase transformations of surfaces investigated.

GEORGIA INSTITUTE OF TECHNOLOGY (continued)

356. INVESTIGATIONS OF INTERMETALLIC ALLOY HYDRIDING MECHANISMS — $ 60,000 — 01-1
B. R. Livesay - Applied Science Laboratory
Phone: (404)-894-3489

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

UNIVERSITY OF HOUSTON

357. MICROSTRUCTURAL STUDIES OF HYDROGEN AND OTHER INTERSTITIAL DEFECTS IN BCC REFRACTORY METALS — $ 77,300 — 02-2
S. C. Moss - Dept. of Physics
Phone: (713)-749-2840

X-ray and neutron diffraction analyses of order-disorder transitions, phase changes, and occupancy sites of H_2 and D_2 in BCC refractory metals -- Nb, Ta, V; anomalous solubility of H_2 in V-Nb solid solutions; interstitial-induced strain fields and Fermi surface modifications; order-disorder transitions in the K distribution in intercalated graphite.

ILLINOIS INSTITUTE OF TECHNOLOGY

358. DIFFUSION MECHANISMS AND DEGRADATION OF ENVIRONMENTALLY SENSITIVE COMPOSITE MATERIALS — $ 45,968 — 01-2
L. J. Broutman - Dept. of Metallurgy and Materials Engineering
Phone: (312)-567-3049

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

359. ELECTROCHEMISTRY OF ACETYLIDES, NITRIDES AND CARBON CATHODES IN MOLTEN HALIDES — $ 66,000 — 03-3
J. R. Selman - Dept. of Chemical Engineering
Phone: (312)-567-3037

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

JOHNS HOPKINS UNIVERSITY

360. CONDENSATION PROCESSES IN COAL COMBUSTION PRODUCTS — $ 63,000 — 03-3

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

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

UNIVERSITY OF KENTUCKY

361. STUDIES OF THE MICROSCOPIC PHYSICAL AND CHEMICAL PROPERTIES OF GRAPHITE INTERCALATION COMPOUNDS — $ 68,335 — 02-2

P. C. Eklund - Dept. of Physics and Astronomy
Phone: (606)-258-4849

Highly oriented pyrolytic graphite (HOPG) will be intercalated with SbX_5 or SbX_3Y_2 where X and Y are halogens. Alkali metal hydride intercalates will also be made. Materials will be studied by optical reflectance, Mössbauer spectroscopy, X-ray diffraction, Shubnikov de Haas effects, magnetoresistance, Raman and infrared spectroscopy.

362. ANISOTROPIC ELASTICITY OF COAL — $ 68,950 — 01-2

Peter P. Gillis - Dept. of Metallurgical Engineering and Materials Science
Phone: (606)-258-5733, 8883
Anthony B. Szwilski - Dept. of Civil Engineering
Phone: (606)-258-2953, 4856

Investigations of the anisotropic elastic constants of coal. Static and dynamic measurements are performed and attempts to relate the results to the structure of the various coals being studied are being made. Objectives include the development of coal-sample preparation/selection procedures that lead to meaningful and reproducible research results.

LEHIGH UNIVERSITY

363. ANALYTICAL STUDY OF DRAWING AND EXTRUSION OF SUPERCONDUCTING FILAMENTARY WIRE: FRACTURE PROBLEMS AND EVALUATION OF TEMPERATURE RISE — $ 89,852 — 01-5

B. Avitzur - Dept. of Metallurgy and Materials Engineering
Phone: (215)-861-4233
Y. T. Chou - Dept. of Metallurgy and Materials Engineering
Phone: (215)-861-4235

Analytical bases for extrusion and drawing processes in the fabrication of multifilament superconducting wire; analyses/understanding of failure modes, viz., central burst phenomena and temperature increases during deformation; electrical properties of finished superconducting wires; Nb_3Sn.

364. AN EXPERIMENTAL AND ANALYTICAL INVESTIGATION OF THE CREEP-RUPTURE PROCESS — $ 59,200 — 01-2

T. Delph - Dept. of Mechanical Engineering and Mechanics
Phone: (215)-861-4119

Experimental and modelling study of creep in austenitic stainless steels under uniaxial and multiaxial stress states; measurement of cavitation kinetics; analysis of cavity linkage.

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

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

The purpose of the proposed research is to compare densification behavior during hot-pressing with deformation during creep; the major goal is to better understand the relation between these two processes and to develop quantitative modeling between them. Concerns are: (1) Grain growth studies on theoretically dense hot isostatically pressed CoC; this is being combined with previous work on grain growth in CoO with about 2 percent porosity in order to examine both grain growth in a dense medium and the effect of porosity on the magnitude and kinetics of grain growth, (2) Microstructure development in pure and impurity doped CoO and NiO in order to study the effect of impurity additions of Cr and Ti upon the pore-pinch-off behavior, and (3) Grain boundary segregation and precipitation studies in Cr doped NiO, using STEM equipped with an X-ray microanalyzer, in order to relate the spatial distribution of impurity additives to the microstructural effects.

LOUISIANA STATE UNIVERSITY

366. INTER-SUBBAND OPTICAL ABSORPTION IN AN INVERSION LAYER ON A SEMICONDUCTOR SURFACE IN TILTED MAGNETIC FIELDS — $ 55,619 — 02-3

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

Theoretical investigations of Faraday rotation and other magneto-optical phenomena in metal-oxide-semiconductor (MOS) systems. The influence of electron-electron coupling and multiple reflection effects in MOS systems will be investigated. The implications arising from recent evidence of a crystallized ground state in silicon inversion layers and the effect of a magnetic field on various many-body effects will be pursued.

UNIVERSITY OF MARYLAND

367. ADSORPTION ON METAL SURFACES — $135,020 — 02-2

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

Joint theoretical/experimental study of surface interactions which, though they involve small characteristic energies, have a significant influence on surface reactivity. Investigation of the molecular precursor state of oxygen on thin film and fully-characterized single crystal metal surfaces; identification of the physical nature of the activation barrier. Study of adatom-adatom interactions using high-resolution LEED/Auger to examine long- and short-range order of chemisorbed layers; Monte-Carlo simulations of phase diagrams will be made to obtain interaction parameters. Experimental determinations of critical exponents associated with two-dimensional phase transitions and comparison with phase-transition theory.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

368. MICROMECHANICAL MODELLING OF MICROSTRUCTURAL DAMAGE AT ELEVATED TEMPERATURE DURING CREEP OF SUPER-ALLOYS FOR ENERGY APPLICATIONS — $146,000 — 01-2

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

Analysis of creep cavitation and cracking in metals, principally austenitic stainless steels; modelling of stress and strain concentrations at particles on grain boundaries and their influence on local deformation and cavitation; calculation of cavity growth in diffusion vs deformation controlled strain fields; measurement of cavity growth kinetics; stress distribution around boundary particles and at triple junctions; relaxation processes around a macroscopic crack tip.

369. STRUCTURE AND PROPERTIES OF GRAIN BOUNDARIES — $245,255 — 01-1

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

Grain boundaries in metals and ceramics; experimental, theoretical and computer simulation; computer simulation of intrinsic structures of grain boundaries and grain boundary dislocations; computer simulation of the structure and energy of point defects in grain boundaries; investigation of various grain boundary models using computer simulation and physical modeling; effect of thermal energy on grain boundary structure and diffusional processes; experimental study of grain boundary energy versus misorientation for [001] twist boundaries in MgO; volume dependence of grain boundary energy; diffusion induced grain boundary migration; fabricated bicrystals of Au and Ag.

370. INTERFACIAL AND COLLOIDAL ASPECTS OF AQUEOUS SUSPENSIONS CONTAINING OXIDIC POWDERS — $ 60,000 — 01-5

A. Bleier - Dept. of Materials Science and Engineering
Phone: (617)-253-6877

Application of colloid-chemical models of single oxides to the processing of their powders. Extension of such models to heterogeneous systems containing more than one particle (composition) type, so as to improve understanding of interfacial complexation and related phenomena which influence dispersibility and packing behavior. Objectives include preparation of model, colloidal single and multimetallic oxides using established synthesis routes, characterization of these oxides using crystallographic, chemical, physical, and surface-chemical procedures, and evaluation of the Davis, James and Leckie model of the electrical double layer.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

371. PHYSICS AND CHEMISTRY OF PACKING FINE CERAMIC POWDERS — $100,000 — 01-5
H. Kent Bowen - Dept. of Materials Science and Engineering
Phone: (617)-253-6892

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

372. BASIC RESEARCH IN CRYSTALLINE AND NONCRYSTALLINE CERAMIC SYSTEMS — $585,000 — 01-1
W. D. Kingery - Dept. of Materials Science and Engineering
Phone: (617)-253-3319
R. L. Coble - Dept. of Materials Science and Engineering
Phone: (617)-253-3318

Broad program on the science of ceramic materials; MgO used as a model material; electrical, optical, dielectric properties; defect structure, kinetics, sintering and creep studies; ionic conductivity and Mg vacancy mobility in MgO; boron diffusion in SiC; characterization of grain boundary segregation in MgO; sintering of covalent (Si) materials; influence of grain size distributions and grain arrangements on grain boundary diffusion creep; STEM studies of grain boundary composition; hot stage SEM study of microstructure development; rapid quenching of solid ceramic samples; breakaway grain growth in MgO doped Al_2O_3.

373. LOW TEMPERATURE AND NEUTRON PHYSICS STUDIES — $158,936 — 02-1
C. G. Shull - Dept. of Physics
Phone: (617)-253-4521

Fundamental experiments in neutron diffraction and interferometry using the MIT research reactor, such as the analogue of the famous optical Fizeau experiment in which fringe shifts are observed when light is sent through a moving medium; neutrons which enter a crystal at an exact Bragg angle propagate through the crystal along the Bragg planes at a drift velocity which is much less than the group velocity. Ways are being sought to exploit this effect. Ways are also being sought to use neutron interferometry to test nonlinear variants of wave mechanics. Effect of interferometer rotation; nature of coherent wave front in interferometer; single and multiple slit Fresnel diffraction patterns.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

374. SPECTROSCOPIC INVESTIGATIONS OF SMALL MOLECULE INTERACTIONS ON METAL OXIDE SURFACES — $ 75,000 — 03-1

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

Studies of the interaction of CO with a variety of low index ZnO surfaces, using both angular-resolved and angular-integrated UV photoemission. Derivation of alignment of CO with selected ZnO surfaces, and measurements of relative CO coverage and displacement by NH_3.

375. A BASIC STUDY OF HEAT FLOW IN FUSION WELDING — $ 89,500 — 01-5

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

Modelling and confirmatory experiments of electroslag and arc welding processes; grain coarsening in the heat affected zone with electroslag welding; importance of initial grain size, heat input, and accelerated cooling on coarsening; effect of spatial distribution of the heat flux in arc welding on the heat affected zone width; plasma temperature and velocity profiles in arc welding; material-low alloy steels.

376. HIGH TEMPERATURE PROPERTIES AND PROCESSES IN CERAMICS: THERMOMIGRATION — $ 68,000 — 01-3

B. J. Wuensch - Dept. of Materials Science and Engineering
Phone: (617)-253-6889

Effects of large temperature gradients on atomic transport behavior, defect structure, and resulting physical properties of ceramics such as KCl, UO_2, FeO, and MgO solutions. Study of principles of atomic transport due to driving forces other than composition gradients by: (a) experiments on well-defined systems with measurable boundary conditions, (b) analysis and solutions of thermomigration relations for the time dependent case, (c) examination of the assumption of local electrochemical equilibrium during the transport processes, and (d) separating the coupling coefficient into well defined kinetic and thermodynamic terms and into those which are truly reversible in nature.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY (continued)

377. FUNDAMENTAL INVESTIGATIONS OF THE OXIDATION OF ALLOYS IN MULTICOMPONENT GASEOUS ENVIRONMENTS — $ 79,100 — 01-3

G. J. Yurek - Dept. of Materials Science and Engineering
Phone: (617)-253-3239

Oxidation of Cr and Fe-Cr alloys in gases over a range of O:S potentials; differences in Cr_2O_3 formation kinetics and structure depending upon substrate crystallography; techniques used--thermogravimetry, STEM, SAM.

UNIVERSITY OF MASSACHUSETTS

378. SYNTHESIS OF METASTABLE A-15 SUPERCONDUCTING COMPOUNDS BY ION IMPLANTATION AND ELECTRON BEAM MELTING — $ 43,000 — 02-2

M. T. Clapp - Dept. of Mechanical Engineering
Phone: (413)-545-0868

Synthesis of metastable A-15 compounds by replacement of deficient compounds via programmed ion implantation to achieve stoichiometry. The resulting material is subsequently heat treated to anneal out radiation damage and to recrystallize the A-15 structure. Compounds to be produced include Nb_3B and Nb_3C. Correlations of the superconducting properties with compositional, structural and thermal processing parameters will be made.

379. EROSION OF STRUCTURAL CERAMICS — $ 46,600 — 01-5

J. E. Ritter, Jr. - Dept. of Mechanical Engineering
Phone: (413)-545-0632
K. Jakus - Dept. of Mechanical Engineering
Phone: (413)-545-2424

Erosion behavior and related strength degradation of Al_2O_3, Si_3N_4, and SiC to 1200°C. Assessment of erosion models for predicting erosion behavior and associated strength degradation. Effect of eroding particle velocity, size, angle of impingement, temperature of environment, and subcritical crack growth on erosion rate and related strength degradation for Al_2O_3, SiC, and Si_3N_4.

MICHIGAN STATE UNIVERSITY

380. STUDIES ON AGE-HARDENING IN SPINODALLY MODULATED ALLOYS - EXPERIMENTAL AND THEORETICAL — $ 55,362 — 01-2

K. N. Subramanian - Dept. of Metallurgy, Mechanics and Materials Science
Phone: (517)-355-2211
M. Kato - Dept. of Metallurgy, Mechanics and Materials Science
Phone: (517)-355-0294

Structure-property relationship and age-hardening mechanism of the spinodal alloy system Cu-10%Ni-6%Sn. Single crystal studies of mechanical properties of both one dimensionally and three dimensionally modulated alloys. Dislocation mobility studies by in-situ TEM (with deformation stage) experiments. Application and development of elasticity and hardening theories to various multi-phase morphologies associated with the spinodal decomposition reaction. Computer analysis of the energetics of dislocation double-kink formation and for thermally activated dislocation motion. Experiments and theory concerning temperature and strain-rate dependent mechanical behavior.

MICHIGAN TECHNOLOGICAL UNIVERSITY

381. ENVIRONMENT-INDUCED EMBRITTLEMENT: EFFECTS OF IMPURITY SEGREGATION AND STATE OF STRESS — $ 75,000 — 01-2

L. A. Heldt - Dept. of Metallurgical Engineering
Phone: (906)-487-2630
D. A. Koss - Dept. of Metallurgical Engineering
Phone: (906)-487-2170

Hydrogen embrittlement and stress corrosion cracking behavior, and the role of grain boundaries, multiaxial stress and strain states, and microstructural variables on such behavior. Hydrogen grain boundary transport in bicrystals of Ni. Effect of H on tensile behavior and local plastic strain. Testing of gridded sheet specimens and application of sheet metal plasticity analysis.

Stein - 906 487 2200

UNIVERSITY OF MICHIGAN

382. SURFACE-PLASMON EXPLORATION OF MULTILAYER PHYSISORBED AND CHEMISORBED FILMS ON METAL SUBSTRATES — $ 63,594 — 02-2

M. Bretz - Dept. of Physics
Phone: (313)-764-4494

Measuring the dielectric properties of adsorbed films by means of the loss associated with surface plasmon excitations, one can study submonolayer to multilayer adsorbed gas films and hence probe a variety of phenomena in two and three dimensions. Measurements will be made on both noble gas films and nonspherical molecules such as CO on metals where orientation effects should be easily detectable.

383. EFFECT OF CRYSTALLIZATION OF GRAIN BOUNDARY PHASE ON THE HIGH TEMPERATURE STRENGTH OF SILICON NITRIDE CERAMICS — $ 61,753 — 01-1

T. Y. Tien - Dept. of Materials and Metallurgical Engineering
Phone: (313)-764-9449

Study of role and mechanism of nucleating agents on the crystallization of the Si_2N_2O containing grain boundary phases which are formed during the processing of Si_3N_4 (containing Y_2O_3 and Al_2O_3) and SIALON ceramics. Microstructure and phase identification in sintered and hot pressed specimens. X-ray diffraction, scanning transmission electron microscopy, electron energy loss spectroscopy, fractography analysis.

Stanford

UNIVERSITY OF MINNESOTA

384. NEAR NEIGHBOR SEPARATIONS OF SURFACE ATOMS — $ 51,115 — 02-2
P. I. Cohen - Dept. of Electrical Engineering
Phone: (612)-373-3025

Techniques are being developed to determine the nearest neighbor distances of atoms at the surfaces of solids by measurement of the extended fine structure in the excitation probability of core level electrons by an incident electron beam. Study will be initially made of oxygen on a Ni(111) surface in order to test the method.

385. A MICROSTRUCTURAL APPROACH TO FATIGUE CRACK PROCESSES IN POLYCRYSTALLINE BCC MATERIALS — $ 68,454 — 01-2
W. W. Gerberich - Dept. of Chemical Engineering and Materials Science
Phone: (612)-373-4829

Investigation of deformation-fracture-microstructure interrelationships in fatigue of Fe, Fe-Si alloys, high strength low alloy steels, and Ti-30 Mo; influence of mechanical properties--strain rate sensitivity, flow stress and its temperature dependence, and monotonic vs cyclic loading; effects of microstructural features such as grain size and slip characteristics; analysis of cyclic strain hardening exponent and ductile-brittle transition temperature; modelling in terms of dislocation dynamics and fracture toughness parameters; techniques used: electron channeling, TEM, SEM.

386. EXPERIMENTAL STUDY OF THE THERMODYNAMICS OF THIN FILMS AND SURFACES — $ 99,000 — 02-2
A. M. Goldman - School of Physics
Phone: (612)-373-5480
E. D. Dahlberg - School of Physics
Phone: (612)-373-3358

Development of a calorimeter especially suited to the study of the heat capacities of extremely thin films. Integrated circuit techniques which have been used to fabricate single-crystal silicon membrane Josephson tunneling junctions will be applied. If successful, the calorimeter will be used to study inversion layers of Si-MOS structures and phase transitions of monolayers on silicon single crystals. Auger spectroscopy and LEED used to study structure of adsorbent and adsorbate.

Stanley L 612-373-2955

UNIVERSITY OF MINNESOTA (continued)

387. FAR INFRARED AND THERMAL STUDIES ON LOW TEMPERATURE MATERIALS — $ 63,335 — 02-2

Cheng-cher Huang - School of Physics and Astronomy
Phone: (612)-373-3787

A combined spectroscopy and thermal properties study of various superconducting systems: A15's, Chevrel phases and rare earth rhodium borides and superionic conductors. Modulated far infrared spectroscopy in both transmission and absorption will be used to determine the electron-phonon coupling and gap parameter.

388. CORROSION RESEARCH CENTER — $950,000 — 01-1

R. Oriani - Dept. of Chemical Engineering and Materials Science
Phone: (612)-373-4864

Research and technology transfer in corrosion; multidisciplinary approach to corrosion research; theory of solid-fluid interfaces; plasma-sprayed coatings; adhesion of polymeric coatings; laser surface modification; plasma-processed polymer coatings; the healing process at polymer-polymer interfaces; desorption of H_2 as a chemical probe of the partial oxidation of Zn surfaces; corrosion fatigue of iron and titanium alloys; hydrogen trapping in titanium alloys; stress corrosion resistance of polymer glasses containing a rubber-reinforced ductile phase; stress corrosion cracking of electroslag refined 316 stainless steel; protection of surfaces via covalent organometallic transition metal complexes; infrared laser-induced reactions at solid-gas interfaces; reduction and cycling fatigue of oxide films; measurements of the oxidation state of iron in thin films with Auger electron and X-ray spectroscopy.

UNIVERSITY OF MISSOURI

389. DEVELOPMENT AND CHARACTERIZATION OF HIGH TEMPERATURE ELECTRICALLY CONDUCTING OXIDES — $100,000 — 01-3

H. E. Anderson - Dept. of Ceramic Engineering
Phone: (314)-341-4401
C. A. Sorrell - Dept. of Ceramic Engineering
Phone: (314)-341-4403

Interrelationship of electrical conductivity, oxidation-reduction kinetics, defect structure, and composition for n type transition metal oxides TiO_2, $SrTiO_3$, and $BaTiO_3$, and p type transition metal oxides Cr_2O_3, NiO, $LaCrO_3$, and $YCrO_3$. Experimental aspects include specimen preparation, thermogravimetric measurements, X-ray diffraction, transmission electron microscopy, and magnetic susceptibility, Hall, conductivity, and Seebeck measurements.

UNIVERSITY OF MISSOURI (continued)

390. ELECTRONIC PROPERTIES OF AMORPHOUS SILICON DIOXIDE AND METALLIC IONS IN SILICATE GLASSES — $ 28,000 — 01-1
W-Y. Ching - Dept. of Physics
Phone: (816)-276-1604

Theoretical study of the electronic properties of amorphous SiO_2, SiO_x, silicon based ceramic crystals, silicate glasses and impurity ions and defect centers in glasses. Combination of computer modelling for structures and quantum mechanical calculation of electron states by first principles OLCAO method. Energy band structures and density of states of crystalline SiO_2, β-Si_3N_4 and α-Si_3N_4 using the OLCAO method; electronic structure of Si_3N_4 from a first principles approach; quasi-periodic structural models of a-SiO_2 and SiO_x and their radial distribution functions; oxygen impurity states in an environment of amorphous Si. The latter is part of a general study of defect states and bonding configuration in a-Si which bears direct resemblance to defect states in glasses. Development of theoretical methods and computer codes for self consistent calculations within the framework of direct space LCAO method.

NEW MEXICO INSTITUTE OF MINING AND TECHNOLOGY

391. MICROSTRUCTURAL AND MECHANICAL PROPERTY STUDY OF SOLAR ENERGY COLLECTORS — $ 83,286 — 01-1
O. T. Inal - Dept. of Metallurgical and Materials Engineering
Phone: (505)-835-5229

Effect of plating geometry, bath compositions and current densities on the surface structure of electroplated black Cr_2O_3 and anodic oxidation of leaf Zn, Zn electroplated steel, and hot-dip galvanized steel. TEM, FIM, nucleation, solar absorption, thermal cycle, and mechanical adhesion studies.

CITY UNIVERSITY OF NEW YORK, BROOKLYN COLLEGE

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

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

CITY UNIVERSITY OF NEW YORK, CITY COLLEGE

393. MELTING PHENOMENA INVESTIGATED BY LASER LIGHT SCATTERING — $172,261 (2 years) — 02-2
H. Z. Cummins - Dept. of Physics
Phone: (212)-690-6921

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

394. CRITICAL CONDITIONS FOR THE GROWTH OF SiC, Si_3N_4, and SiO_2 — $ 56,472 — 01-5
F. W. Smith - Dept. of Physics
Phone: (212)-690-6963

Critical conditions for chemical vapor deposition growth of films of SiC, Si_3N_4, and SiO_2 on single crystal Si substrate are studied under ultrahigh vacuum conditions, and the high temperature interactions of C_2H_2, C_2H_4, CH_4, CO, NH_3, N_2, NO, O_2, and H_2O with clean (111) and (100) surfaces of Si are investigated. Oxide and carbide film formation on polycrystalline W, Mo, and Ta substrates, with partial pressure of reactants and substrate temperature as controlled variables. Analytical techniques include electron spectroscopy for chemical analysis, Auger electron spectroscopy, secondary ion mass spectroscopy, infrared absorption, X-ray diffraction, and scanning electron microscopy.

POLYTECHNIC INSTITUTE OF NEW YORK

395. PHOTOEMISSION STUDIES OF f-ELECTRON SYSTEMS: MANY BODY EFFECTS — $ 60,000 — 02-2
R. D. Parks - Dept. of Physics
Phone: (212)-643-2070

Study of mixed valence, cerium based alloys such as $Ce_{0.9-x}La_xTh_{0.1}$ by time resolved X-ray photoemission spectroscopy. Study of well characterized mixed valent systems which exhibit valence transitions with temperature and have various 4f-(5d,6s) hybridization strengths to study many body screening effects observed frequently in deep level photoemission.

STATE UNIVERSITY OF NEW YORK/STONY BROOK

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

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

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

397. SYNCHROTRON TOPOGRAPHIC PROJECT PARTICIPATING RESEARCH TEAM — $380,000 — 01-1

J. C. Bilello - Dept. of Materials Science and Engineering
Phone: (516)-246-6750/6751
J. M. Liu - Dept. of Materials Science and Engineering
Phone: (516)-246-5983

Synchrotron X-ray diffraction topography to investigate plastic flow under multiaxial stresses and characterize the deformed solid state, hydrogen related fracture, hydrogen attack, hydride formation, protective oxide films, microradiography of voids, crystal growth and phase transitions in Heusler alloys, dislocations generated by the decomposition of pseudostable solid inorganic compounds, ion implantation, internal stress and strain distributions within superconductors, and nondestructive testing with an asymmetric crystal topographic camera and real time detectors.

398. SURFACE STUDIES: A PROPOSAL FOR PARTICIPATING RESEARCH TEAM AT NSLS — $242,236 (20 months) — 02-2

F. Jona - Dept. of Materials Science and Engineering
Phone: (516)-246-7649/6759

Development of a versatile, high-vacuum experimental chamber for surface research with the VUV ring at NSLS; chamber will include LEED, Auger, and photoemission facilities. Studies of atomic structure of solid surfaces: Al, Fe, and Ti, both clean and with O, S, Cl, and CO adsorbates; SEXAFS. Chemisorption, physiosorption and hydrogen uptake: H uptake by Nb; O on Ni and Nb; Pd on Nb and Ta. Electronic properties of solids: lifetimes of excited states in metals and insulators; effects of bulk phase transitions on surface structure; surface and bulk properties of FeTi.

NORTH CAROLINA STATE UNIVERSITY

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

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

Development of an advanced EXAFS beam line at NSLS for a Participating Research Team (PRT) with members from North Carolina State University, University of Connecticut, University of Washington, University of Delaware, Brookhaven National Laboratory, United Technologies, and General Electric. Facility will cover the energy range from ∿1 to ∿20 keV and include provisions for transmission EXAFS, fluorescence EXAFS, SEXAFS, and X-ray absorption studies other than those associated with EXAFS. Wide-ranging materials science research program: metallurgy, corrosion, amorphous materials, catalysis, surface science, electrochemistry, magnetic properties.

UNIVERSITY OF NORTH CAROLINA

400. THE STRUCTURE OF NEUTRON DAMAGE IN IONIC REFRACTORY OXIDES — $ 59,136 — 01-4

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

Structure, thermal stability, and influence of charge state upon the behavior of lattice defects created by fast neutron bombardment and thermo-chemical treatment in refractory oxide single crystals. Experimental probes used to explore defect structure include optical absorption spectroscopy over the spectral range from vacuum ultraviolet to infrared, luminescent emission as excited by photons and ionizing radiation (X-rays and electron pulsed in the nsec region to permit time resolved spectroscopy), electron spin resonance, dimensional change measurements in the 10^{-6} range, electrical conductivity and electrical polarization measurements by both thermal depolarization and dielectric loss as a function of temperature. Materials under investigation include MgO, Al_2O_3, $MgAl_2O_4$, $Y_3Al_5O_{12}$, and TiO_2.

NORTHEASTERN UNIVERSITY

401. DYNAMICAL FRICTION IN CONDENSED MATTER — $ 78,494 — 02-3

J. B. Sokoloff - Dept. of Physics
Phone: (617)-437-2931
C. H. Perry - Dept. of Physics
Phone: (617)-437-2913

Joint theoretical-experimental studies of a variety of systems reflecting motion of one set of species (ions, defects, layers) relative to another set of species (channels, lattices, layers). The rate of energy dissipation, its frequency and temperature dependence will be calculated as well as electronic contributions to the damping. Experimental studies of yttria, zirconia, hollandite, intercalated calcogenides will be related to the theoretical models, including a predicted electric field effect.

NORTHWESTERN UNIVERSITY

402. INVESTIGATION OF DISPERSED IRON ALLOY CATALYSTS IN THE CARBON MONOXIDE-HYDROGEN SYNTHESIS REACTION — $ 97,942 — 01-3

J. B. Butt - Dept. of Chemical Engineering
Phone: (312)-492-7620
L. H. Schwartz - Dept. of Materials Science and Engineering
Phone: (312)-492-3606

Preparation, characterization and catalytic behavior of binary iron alloy catalysts supported on silica substrates for the CO-H_2 synthesis reaction; catalyst systems: Fe-Ni, Fe-Co, Fe-Cu, Fe-K and Fe-N; characterization of catalyst particle sizes and phases using X-ray diffraction, transmission electron microscopy and Mossbauer spectroscopy; reaction studies.

403. STUDIES OF METAL-SEMICONDUCTOR INTERFACES IN CATALYSIS AND ENERGY CONVERSION — $ 85,000 — 03-1

Y-W. Chung - Dept. of Materials Science and Engineering
Phone: (312)-492-3112

Studies of catalyst-support interactions in methanation catalysis, with emphasis on chemical states of ad-atoms on semiconductor surfaces using X-ray photoemission. Measurement of the chemical states of Ni atoms dispersed on TiO_2(110) surfaces that have been prepared to give different surface oxygen-to-titanium ratios. Correlation between electron transfer from TiO_2 to Ni and O/Ti ratio on the TiO_2 surface; gas phase photo-decomposition of water.

404. EFFECT ON POINT DEFECTS ON MECHANICAL PROPERTIES OF METALS — $ 73,772 — 01-2

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

Experimental and analytical investigation of low temperature flow behavior of Nb; influence of crystallographic orientation and interstitial atoms on deformation by primary vs anomalous slip; effects of H_2 charging on dislocation motion and low temperature softening of Fe as well as on fracture by quasicleavage, microvoid coalescence, or a brittle intergranular mode.

NORTHWESTERN UNIVERSITY (continued)

405. AN INVESTIGATION OF MICRO-STRUCTURAL CHANGES IN FERRITIC STAINLESS STEELS CAUSED BY HIGH TEMPERATURE DEFORMATION — $ 63,680 (14 months) — 01-2
J. R. Weertman - Dept. of Materials Science and Engineering
Phone: (312)-492-5353

Investigation of creep and creep-fatigue in low alloy ferritic steels; TEM and SANS characterization of strain and thermal induced microstructural modifications, e.g., carbide precipitation, cavity formation.

406. INVESTIGATION OF DEEP LEVEL DEFECTS IN EPITAXIAL SEMICONDUCTING ZINC SULPHO-SELENIDE — $ 53,234 — 01-3
B. W. Wessels - Dept. of Materials Science and Engineering
Phone: (312)-492-3219

Preparation of high purity ZnS_xSe_{1-x} heteroepitaxially deposited by chemical vapor deposition on substrates of ZnSe, GaAs, and Ge. Defect identification and exploration of compensation mechanisms by measuring ionization energies of deep acceptors and donors using deep level transient spectroscopy on deliberately doped n-type and p-type material. Role of misfit dislocations on deep level defects. Optical and electrical modulation of the space charge region. The ternary compound will also be characterized by Hall effect, scanning Auger microscopy, and photoluminescence. Photoresponse of ZnS_xSe_{1-x}/GaAs heterojunctions.

407. BASIC RESEARCH ON CERAMIC MATERIALS FOR ENERGY STORAGE AND CONVERSION SYSTEMS — $ 71,500 — 01-1
D. H. Whitmore - Dept. of Materials Science and Engineering
Phone: (312)-492-3533

Investigation of factors affecting electronic and mass transport behavior in solid electrolyte and electrode materials; study of the effect of a dispersed second (non-soluble) phase on ionic transport in solid electrolytes; synthesis and characterization of new materials which are potential candidates for solid electrodes or electrolytes in energy storage or conversion devices; and optimization of the factors affecting the fabrication and ion transport properties of dense polycrystalline specimens of new solid electrolyte and electrode materials. Experimental effort involves measurements of ac conductivity, dc polarization, tracer diffusion, dielectric loss, and ion thermal current. Experimental techniques include infrared reflectivity, Raman spectroscopy, pulsed field gradient and stimulated echo NMR, and the chemical preparation and crystal growth of selected electrolyte materials. Systems under investigation include protonic conduction in β" aluminas and β" gallates, Na transport in NASICON and sodium antimonate, fast alkali ion conduction in polymer electrolytes, and LiI-SiO_2 composites.

UNIVERSITY OF NOTRE DAME

408. MICROSTRUCTURAL EFFECTS IN ABRASIVE WEAR — $ 88,093 (15 months) — 01-5

N. F. Fiore - Dept. of Metallurgical Engineering and Materials Science
Phone: (219)-283-4516
T. H. Kosel - Dept. of Metallurgical Engineering and Materials Science
Phone: (219)-283-4302

Assessment of mechanisms controlling abrasive wear in multiphase alloys; influence of abrasive hardness and angularity; role of wear debris; in-situ SEM scratch tests; change in near-surface microstructure under abrasive wear conditions.

409. PORE SHRINKAGE AND OSTWALD RIPENING IN METALLIC SYSTEMS — $ 53,000 — 01-1

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

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

OHIO STATE UNIVERSITY

410. INFLUENCE OF NITROGEN ON THE SENSITIZATION, CORROSION, MECHANICAL AND MICROSTRUCTURAL PROPERTIES OF AUSTENITIC STAINLESS STEELS — $ 59,300 — 01-1

W. Clark - Dept. of Metallurgical Engineering
Phone: (614)-422-2538
D. D. Macdonald - Dept. of Metallurgical Engineering
Phone: (614)-422-6255

Evaluation of corrosion and stress corrosion cracking of austenitic stainless steel with various C and N contents; TEM characterization of grain boundary structure as well as carbide and nitride morphologies and distribution; measurement of electrochemical parameters in static and flowing aqueous solutions containing chloride and sulfate ions.

OHIO STATE UNIVERSITY (continued)

411. FUNDAMENTAL STUDIES OF HIGH TEMPERATURE CORROSION REACTIONS — $ 85,600 — 01-1
R. A. Rapp - Dept. of Metallurgical Engineering
Phone: (614)-422-6178

In-situ SEM study of oxidation of metals, initially Cu and Cu-Ni alloys; vapor phase oxide nucleation and screw dislocations growth mechanisms; preferential NiO formation at twin and grain boundaries in Cu-Ni alloys; kinetics of sulfidation of Mo in S_2 and H_2/H_2S mixtures; MoS_2 scale orientation and deformation during growth.

412. HYDROGEN ATTACK OF STEEL — $ 55,000 — 01-2
Paul G. Shewmon - Dept. of Metallurgical Engineering
Phone: (614)-422-2491

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

OREGON STATE UNIVERSITY

413. INVESTIGATION OF THE ELECTRICAL OPTICAL PROPERTIES OF ORGANOMETALLIC VAPOR PHASE EPITAXIAL $Ga_{1-x}Al_xAs$ AND $Ga_{1-x}Al_xAs/GaAs$ INTERFACES IN SOLAR CELLS — $ 73,852 — 01-3
P. K. Bhattacharya - Dept. of Electrical and Computer Engineering
Phone: (503)-754-3617

Electrical and optical characterization of undoped and intentionally doped $Ga_{1-x}Al_xAs$ layers and $Ga_{1-x}Al_xAs/GaAs$ interfaces grown by organo-metallic vapor phase epitaxial growth. Measurements extend over the entire mixed alloy composition range of the ternary alloy with particular emphasis on the indirect bandgap region ($x \geq 0.43$) being used for concentrator heterostructure solar cells. Electrical characterization includes detailed study of deep trapping centers in bulk layers and interface regions and transport properties in these regions as a function of alloy composition and temperature. Optical studies include characteristics of the deep states and luminescence measurements. Measurement techniques are Deep Level Transient Spectroscopy, Double Source Differentiated Photocapacitance, capacitance-voltage, Hall-effect, velocity-field, and photoluminescence.

PENNSYLVANIA STATE UNIVERSITY

414. PHYSICAL ADSORPTION: RARE GAS ATOMS NEAR SOLID SURFACES — $ 26,847 (7 months) — 02-3
M. W. Cole - Dept. of Physics
Phone: (814)-863-0165

Theoretical studies directed to the understanding of interactions associated with physical adsorption and the associated properties of a film. Specific topics to be pursued include the detailed form of the long range interaction, the configuration space wave function, and the interaction between adatoms. Additional studies of the theory of photo-stimulated field emission and phonon reflection at interfaces are addressed. The phonon reflection work is directed toward understanding the role of surface roughness, an important factor in influencing energy transmission across interfaces.

415. LASER PROCESSING OF CERAMICS — $ 62,000 — 01-5
G. L. Messing - Dept. of Materials Science and Engineering
Phone: (814)-865-2262

Studies of single component, multicomponent, and decomposition-reaction laser-particle interactions in fine-particle ceramics. Use of a 10.6 micron CO_2 laser to effect calcination without aggregation, morphological modification of particles, and comminution. Thermodynamic and kinetic assessment of effects of rapid heating on processes in fine-particle ceramics, with concerns for potential melting, metamicitization, vaporization, and microcracking phenomena. Initial studies will be on Al_2O_3 and MgO particles and their precursors.

416. HYDROGEN ABSORPTION IN METALS: A FIELD ION MICROSCOPY STUDY — $ 71,000 — 01-1
H. W. Pickering - Dept. of Materials Sciences and Engineering
Phone: (814)-863-2640

Field ion microscopy study of H_2 trapping and absorption in Fe; also oxide formation as well as Ti-O clustering and segregation at grain boundaries; surface and grain boundary segregation of P and Ti in Fe; quantitative measure of the concentration gradients away from boundaries; cosegregation and clustering of impurities.

PENNSYLVANIA STATE UNIVERSITY (continued)

417. GRAIN BOUNDARY DIFFUSION AND GRAIN BOUNDARY CHEMISTRY OF CR-DOPED MAGNESIUM OXIDE — $ 39,000 — 01-3
V. S. Stubican - Dept. of Materials Science
Phone: (814)-865-9921

Aliovalent impurity diffusion in ionic materials, specifically Cr in MgO; binding energy between impurities and vacancies and grain boundary diffusion in MgO; surface diffusion; techniques used--autoradiography, electron micorprobe, ion beam spectrochemical analysis.

418. STUDY OF FIELD ADSORPTION USING IMAGING ATOM-PROBE FIELD ION MICROSCOPY — $ 49,155 — 02-2
T. T. Tsong - Dept. of Physics
Phone: (814)-865-2813

To study in atomic detail the field adsorption of noble gases and classical molecular gases using the imaging atom probe field ion microscope. Measure the adsorption energy as a function of field on catalytically active group VIII metal surfaces. Mechanism of formation of metal-noble gas complex ions. Photon and electron stimulated field desorption.

419. STRUCTURE OF GLASSES CONTAINING TRANSITION METAL IONS — $ 95,000 — 01-1
W. B. White - Materials Research Laboratory
Phone: (814)-865-1152

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

UNIVERSITY OF PENNSYLVANIA

420. HIGH CONDUCTIVITY PROTON SOLID ELECTROLYTES — $ 81,000 — 03-1

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

Preparation and characterization of a series of solid state protonic conductors, for use in the temperature range of 100-400°C. Determination of conductivities of NH_4+-H+-β aluminas, and studies of the influence of the stabilizing cation. Thermal stability of various compositions to be determined in dry and hydrated atmospheres, using TGA and DTA techniques.

421. STUDIES RELATING TO THE HIGH CONDUCTIVITY OF INTERCALATED GRAPHITE — $106,280 — 02-2

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

Synthesize various stages of Ba-intercalated graphite, particularly the stage one material BaC_6. Obtain the chemical structures of these materials, determine the stoichiometries, measure the conductivities and optical properties, and interpret the results in terms of structure and bonding properties. Prepare graphite intercalation compounds using intercalates having a wide range of fluorinating strength (XeF_6, XeF_4, AsF_5, $XeOF_4$, XeF_2), and oxidants such as H_2SO_4. Determine the chemical character and physical properties of these compounds using a number of techniques (NMR, XPS, IR spectroscopy, Raman scattering, paramagnetic resonance, and optical spectroscopy).

422. MECHANISMS OF DAMAGE ACCUMULATION IN TIME DEPENDENT CYCLIC DEFORMATION — $ 58,000 — 01-2

C. Laird - Dept. of Metallurgy and Materials Science
Phone: (215)-243-6664

Identification of microstructural changes resulting from creep and fatigue deformation of metals, initially Cu and low alloy steels; correlation of substructure development with strain hardening and softening during prior monotonic, interrupted, or reversed stress cycles; strain burst occurrence and relationship to substructure instability; technique used - TEM.

UNIVERSITY OF PENNSYLVANIA (continued)

423. ATOMISTIC STUDIES OF GRAIN BOUNDARIES WITH SEGREGATED IMPURITIES — $ 65,100 — 01-1

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

Atomistic-based computer simulation of grain boundary structure in dilute binary metal alloys, initially Au-Ag, Cu-Ag, and Cu-Bi; development of semi-empirical interatomic potentials incorporating charge transfer and atomic volume, and fitted to satisfy lattice parameter and cohesive energy requirements; influence of degree of segregation and boundary periodicity; computation of stress fields around impurities at grain boundaries.

424. ELECTROCHEMICAL INVESTIGATION OF NOVEL ELECTRODE MATERIALS — $ 90,000 — 03-2

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

Intercalation of Na and Li into Li_xTiS_2 and Li_xTaS_2, resulting in increased electrical capacity of cathode materials for advanced batteries. Electrochemical studies of electrode performance, and X-ray structural determination of intercalated compounds. Measurement of diffusion coefficient of Li ions; studies of effect of ionic size and charge on stability of intercalant in the TiS_2 lattice.

UNIVERSITY OF PITTSBURGH

425. HIGH TEMPERATURE CORROSION OF CERAMICS — $ 61,000 — 01-3

F. S. Pettit - Dept. of Metallurgical and Materials Engineering
Phone: (412)-624-5300
J. R. Blachere - Dept. of Metallurgical and Materials Engineering
Phone: (412)-624-5296

Analyses of gaseous and molten salt corrosion of oxides (SiO_2, Al_2O_3, Cr_2O_3, and ZrO_2) in oxidizing, sulfidizing, and reducing environments; thermogravimetric measurement of corrosion kinetics.

PRINCETON UNIVERSITY

426. CHEMICAL POISONING IN HETEROGENEOUSLY CATALYZED REACTIONS — $120,000 (2 years) — 03-1

S. L. Bernasek - Dept. of Chemistry
Phone: (609)-452-4986

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

PURDUE UNIVERSITY

427. ZERO-FLUX PLANES AND FLUX REVERSALS IN MULTICOMPONENT SYSTEMS — $ 64,119 — 01-3

M. A. Dayananda - School of Materials Engineering
Phone: (317)-494-8629

Interdiffusion fluxes of all components in an n-component system are calculated directly from the concentration profiles of a single diffusion couple at any section without invoking Fick's Law or the need for prior knowledge of $(n-1)^2$ interdiffusion coefficients. These studies have identified "zero-flux planes" (ZFP) for individual components, which are planes where the interdiffusion flux of a given component is zero and exhibits reversal in its flow direction on either side of the plane. Objectives include characterization of the ZFP compositions in terms of diffusion paths and thermodynamic data for multicomponent systems.

428. FORMATION OF A PARTICIPATING RESEARCH TEAM AND THE INSTRUMENTATION FOR X-RAY DIFFRACTION AT THE NATIONAL SYNCHROTRON LIGHT SOURCE — $346,000 (14 months) — 01-1

G. L. Liedl - School of Materials Engineering
Phone: (317)-494-4094

Development of an instrumented beam line and port at NSLS for conducting X-ray crystallography/diffuse scattering experiments on a variety of materials: catalysts, dilute metal alloys, non-stoichiometric oxides, intermetallic compounds, plastically deformed region ahead of stable crack, among others.

PURDUE UNIVERSITY (continued)

429. STUDY OF ELECTRONS PHOTO-EMITTED FROM FIELD EMISSION TIPS — $ 50,000 — 01-3

R. Reifenberger - Dept. of Physics
Phone: (317)-493-9318/494-4799

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

430. MULTICOMPONENT DIFFUSION UNDER GENERAL CHEMICAL POTENTIAL GRADIENTS — $ 74,886 — 01-3

Hiroshi Sato - School of Materials Engineering
Phone: (317)-749-2855
Ryoichi Kikuchi - School of Materials Engineering
Phone: (213)-456-6411

Application of the pair approximation of the Path Probability Method (PPM) of time dependent cooperative phenomena to analytically derive the kinetic matrix of Onsager equations from thermodynamic potentials, and some fundamental kinetic parameters such as jump frequencies of component atoms during multicomponent diffusion. Relations among measurable quantities and experimental concepts such as diffusion paths and zero-flux planes in multicomponent diffusion experiments, and specific diffusion controlled phenomena in oxides are being investigated.

431. MECHANISMS OF ELEVATED TEMPERATURE RUPTURE IN SINGLE PHASE CERAMICS — $ 50,000 — 01-2

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

Study of elevated temperature stress rupture in well-characterized single phase ceramics in terms of rate contolling mechanisms and microstructural evolution. Experimental techniques consist of (1) tensile creep using constant time stress, (2) internal pressurization of pores with inert insoluble gas and microscopic measurement of pore or cavity growth under known hydrostatic pressure and surface tension driving forces, (3) characterization of initial powder, and (4) dislocation etch pitting. Preliminary studies will be on ZnO and a metallic system, followed by comprehensive studies on a stoichiometric oxide such as MgO or Al_2O_3, and a non-stoichiometric system such as CoO.

RENSSELAER POLYTECHNIC INSTITUTE

432. MOLTEN CARBONATES: MICROWAVE STUDIES OF THE VAPOR STATE — $ 69,000 — 03-3
Charles W. Gillies - Dept. of Chemistry
Phone: (518)-270-6341

Microwave spectroscopic studies of vapor region above electrode compartments in fuel cells employing molten salts as electrolytes. Evaluation of operating parameters and electrolyte compositions.

433. THERMOPHYSICAL PROPERTIES OF INORGANIC POLYSULFIDES — $ 85,000 — 03-2
G. J. Janz - Dept. of Chemistry
Phone: (518)-270-6344

Synthesis of sodium polysulfides and measurements of the enthalpies of fusion, heat capacities, and volume changes on melting. Investigations of the phase-diagram of the Na-S system.

434. PROTECTIVE OXIDE FILMS — $ 75,000 — 01-3
R. K. MacCrone - Dept. of Materials Engineering
Phone: (518)-270-6495
S. R. Shatynski - Dept. of Materials Engineering
Phone: (518)-270-6448

Study of films of the protective metal oxides NiO and Al_2O_3 by both discontinuous and continuous thermogravimetric analysis, thermally stimulated currents, thermoluminescence, and electron paramagnetic resonance, for the purpose of obtaining a more precise understanding of the oxidation process.

435. LOCALIZED CORROSION AND STRESS CORROSION CRACKING BEHAVIOR OF STAINLESS STEEL WELDMENTS — $118,084 — 01-1
W. F. Savage - Materials Division
Phone: (518)-270-6453
D. J. Duquette - Materials Division
Phone: (518)-270-6448

Corrosion of stainless steel weldments and the effect of welding parameters; chloride environments; effect of delta ferrite on localized corrosion; Cr depletion at grain boundaries; synergistic effect of sulfate and chloride ions on initiation and propagation of stress corrosion cracks; role of grain boundary precipitation; TEM and SEM techniques; work to be started on ferritic stainless steels also; role of surface films.

RENSSELAER POLYTECHNIC INSTITUTE (continued)

436. PROPERTIES OF GLASS WITH HIGH WATER CONTENT — $ 84,000 — 01-3

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

The effects of dissolved water upon physical, chemical, and transport properties of select glass compositions containing up to $\sim$ 12 wt. % water. These unusual high water content glasses are prepared under combined pressure-temperature conditions of 3 kbar and 800^{o}C. Radiation effects, chemical durability, diffusion, mechanical strength, ion transport processes, differential thermal analysis, thermogravimetric analysis.

RICE UNIVERSITY

437. ELECTRON SPIN POLARIZATION EFFECTS IN LOW ENERGY ELECTRON DIFFRACTION, ION NEUTRALIZATION AND METASTABLE ATOM DEEXCITATION AT SOLID SURFACES — $157,133 — 02-2

G. K. Walters - Dept. of Physics
Phone: (713)-527-4937
F. B. Dunning - Dept. of Physics
Phone: (713)-527-8101

Will use PLEED (polarized LEED) to study surfaces; e.g., Ni with Te adsorbed and W. with H adsorbed. Spin polarization measurements in conjunction with ion neutralization spectroscopy (INS) and metastable deexcitation spectroscopy (MDS) to study surface electronic structure on magnetic materials such as Ni. Polarized He^{+} beams used for INS and polarized He ($2^{3}S$) neutral beams for MDS.

UNIVERSITY OF ROCHESTER

438. FRACTURE TOUGHNESS PROCESSES — $ 72,000 — 01-2

Stephen J. Burns - Dept. of Mechanical and Aerospace Sciences
Phone: (716)-275-4082

Studies of macrocrack-tip dislocation plasticity and the production of microcracks. Materials under investigation include aluminum alloys, various steels, silicon and a number of oxide ceramics. Types of measurements include (a) dislocation nucleation and structures at the tips of cracks, (b) the relationship between positions of dislocations relative to crack-tips and the stress intensity factor for crack propagation, and (c) transmission electron microscopy of dislocations at crack tips.

UNIVERSITY OF ROCHESTER (continued)

439. DIFFUSIONAL CREEP OF MULTI-COMPONENT SYSTEMS — $ 89,000 — 01-2

J. C. M. Li - Dept. of Mechanical and Aerospace Sciences
Phone: (716)-275-4038

Stress-motivated diffusion; elastic and plastic deformation in ceramic, polymer and metallic materials; techniques - "impression" creep, fatigue, load relaxation, and elastic deformation; relationships between bulk and impression test data; polycrystals and single crystals; laser excited solid-state reactions, plasticity, and diffusion; Al, β-tin, LiF, KBr, PMMA, rubber.

ROCKWELL INTERNATIONAL SCIENCE CENTER

440. SINTERING PHENOMENA OF NON-OXIDE SILICON COMPOUNDS — $ 99,053 — 01-1

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

Identification of the dominant mechanisms occurring during the sintering of silicon nitride alloys with particular emphasis on the mechanisms responsible for the compositional changes and weight losses observed. The approach adopted is to measure weight losses and compositional gradients produced during sintering by volatilization and compare them for different sintering environments. From the volatilization compositional vectors determined in this way, the processes responsible for the volatilization can be ascertained, and suitable buffer powders selected for preventing compositional changes during sintering. The overall goal is to understand the interrelation between phase equilibria, compositional changes, and densification parameters with desired properties and behavior in Si_3N_4 alloys. Phase equilibria. Diffusion. Scanning transmission electron microscopy. Analytical electron microscopy.

441. ACOUSTIC EMISSION SIGNATURE ANALYSIS — $ 96,857 — 01-5

W. Pardee
Phone: (805)-498-4545

Application of acoustic emission to detection of cracking mechanisms in glasses and metals; crack growth in embrittled steels; sustained load cracking of hydrogen embrittled steels; multiple transducer Fourier frequency analysis as a function of geometric parameters and of fatigue crack growth. Results include recommended transducer placement and signal processing techniques.

UNIVERSITY OF SOUTHERN CALIFORNIA

442. ELECTRICAL AND MECHANICAL PROPERTIES OF OXIDE CERAMICS — $ 80,000 — 01-3

F. A. Kröger - Dept. of Materials Science
Phone: (213)-743-6224

Role of donor and acceptor impurities, grain boundaries, porosity, and oxygen fugacity in controlling the ion and electronic transport and the creep behavior on Al_2O_3. Emphasis on delineation between grain boundary and bulk effects, and on the determination of relationship between dopant type and concentration, conditions of sample preparation, and physical behavior.

443. GRAIN BOUNDARY SLIDING AND DEFORMATION MECHANISMS DURING HIGH TEMPERATURE CREEP — $100,000 — 01-2

T. G. Langdon - Dept. of Materials Science and Mechanical Engineering
Phone: (213)-743-2095

Measurement of creep and grain boundary sliding in metals--Al, Mg, and Cu, and their alloys--and in alkali halides--KBr; boundary sliding, stress and temperature dependences, threshold creep stress in precipitation hardened and solid solution strengthened Al-base alloys; boundary migration under monotonic as well as cyclic creep; creep parameters for polycrystalline KBr and relationship to lattice vs dislocation core diffusion.

SOUTHERN ILLINOIS UNIVERSITY

444. METALLIC GLASSES AND NON-EQUILIBRIUM PHASES AS NEW CATALYSTS IN ENERGY CONVERSION SYSTEMS — $ 70,000 — 01-1

W. E. Brower, Jr. - Dept. of Engineering Mechanics and Materials
Phone: (618)-536-2368
G. Smith - Dept. of Chemistry and Biochemistry
Phone: (618)-453-5721

Identification of the catalytic activity of non-equilibrium crystalline and amorphous metals, specifically Pd- and Ni- base alloys and the role of defects thereon; characterization of microstructure and transformation kinetics of rapidly-cooled alloys.

SOUTHWEST RESEARCH INSTITUTE

445. THE STUDY AND MODELLING OF HIGH TEMPERATURE FATIGUE CRACK PROPAGATION IN AUSTENITIC STAINLESS STEELS — $ 40,000 — 01-2

D. L. Davidson - Dept. of Materials Sciences
Phone: (512)-684-5111

In-situ observation of strain fields at crack tips in austenitic stainless steels under creep and creep-fatigue loading, and correlation with microstructural features; techniques used: SEM, electron channeling, and optical stereo imaging.

STANFORD UNIVERSITY

446. SUPERCONDUCTING PROPERTIES OF ELECTRON-BEAM EVAPORATED MATERIALS — $133,675 — 02-2

M. R. Beasley - W. W. Hansen Laboratories of Physics
Phone: (415)-497-0215

This is a study of the high magnetic field properties of superconducting films prepared using electron beam coevaporation techniques. Materials studied are mainly A15 structure compounds such as Nb_xSn and V_xSn where x is near 3. Ternary substitutions such as Al for Sn and Fe for Nb are also of interest. Measurements are made of superconducting parameters, such as T_c and dH_{c2}/dT, as well as other mechanical properties such as strain tolerance, micro-hardness and high temperature ductility are studied as a function of composition and microstructure.

447. PHOTOELECTRONIC PROPERTIES OF II-VI HETEROJUNCTIONS — $156,633 — 01-3

R. H. Bube - Dept. of Materials Science and Engineering
Phone: (415)-497-2534

Energy parameters and transport processes that control the electrical, photoelectronic, and photovoltaic properties of II-VI heterojunctions; preparation of II-VI heterojunctions in film-on-crystal and film-on-film form; n-ZnCdS/p-CdTe, N-ZnSSe/p-CdTe, Cu_2S/CdS, ZnO/CdTe, ITO/CdTe; measurements of J-V curves in dark and light; junction capacitance; surface photovoltage; Schottky-barrier formation; spectral response; diffusion lengths; scanning transmission electron microscopy and high resolution TEM analysis of heterojunction interfaces; lattice resolution; electron microdiffraction; Auger analysis; vacuum evaporation; spray pyrolysis; rf sputter deposition, magnetron sputtering, and chemical vapor deposition, and closed-space vapor transport techniques.

STANFORD UNIVERSITY (continued)

448. MODELLING OF DEFORMATION AND FRACTURE IN HIGH-TEMPERATURE STRUCTURAL MATERIALS — $140,000 — 01-2

A. K. Miller - Dept. of Materials Science and Engineering
Phone: (415)-497-3732
O. D. Sherby - Dept. of Materials Science and Engineering
Phone: (415)-497-2536

Development of quantitative methods of predicting deformation and fracture of metals and alloys subjected to complex histories and environments; computer based constitutive equations for non-elastic deformation, "MATMOD"; interactive solute strengthening in Type 316 stainless steel; roles of forest dislocations and subgrains in isotropic hardening, Type 304 stainless steel; back stresses at large strains and high temperatures, Al and Type 304 stainless steel; strain softening; application of MATMOD equations to 2¼ Cr-1Mo steel; elevated temperature fatigue with hold time in ferritic materials.

449. MECHANISMS AND MECHANICS OF HIGH TEMPERATURE FRACTURE OF MATERIALS — $ 88,700 — 01-2

W. D. Nix - Dept. of Materials Science and Engineering
Phone: (415)-497-4259

Study of creep deformation and cavitation in metals--Al, Cu, Fe, and Ni as well as Cu containing water vapor bubbles; dependence of cavitation nucleation and growth on plastic deformation, surface and grain boundary diffusion; mechanisms controlling breakdown of power law creep at high strain rates; grain boundary segregation effects on creep.

STEVENS INSTITUTE OF TECHNOLOGY

450. STUDIES OF MAGNETISM AND EXCHANGE SCATTERING IN SOLIDS USING SYNCHROTRON RADIATION AND SPIN POLARIZED PHOTOELECTRONS — $180,000 — 02-2

G. M. Rothberg - Dept. of Materials and Metallurgical Engineering
Phone: (201)-420-5269

A synchrotron light source will be used to produce polarized photoelectrons from transition metal ions. The multiplet splitting serves as the polarizer. Spin polarized EXAFS will be used to study instantaneous short-range magnetic order above and below transition temperatures and on surfaces and to study temperature dependence of short range order above transition temperatures.

SYRACUSE UNIVERSITY

451. SURFACE CHARACTERIZATION OF CATALYTICALLY ACTIVE METAL ALLOY AND COMPOUND FILMS — $ 91,500 — 01-1

R. W. Vook - Dept. of Chemical Engineering and Materials Sciences
Phone: (315)-423-3466

Defect structure of thin metal films (Pd/Cu, Cu/NaCl); analysis of Auger line shape of the adsorbate to evaluate the film topography during growth; interfacial dislocations; overgrowth structure and growth mechanisms; techniques used: TEM, AES, RHEED.

UNIVERSITY OF TENNESSEE

452. A COMBINED THERMODYNAMIC STUDY OF NICKEL BASE ALLOYS — $ 87,506 — 01-1

C. R. Brooks - Dept. of Chemical and Metallurgical Engineering
Phone: (615)-974-5427
P. J. Meschter - Dept. of Chemical and Metallurgical Engineering
Phone: (615)-974-6009

Free energy-composition curves for stable and metastable phases in nickel alloy systems as functions of temperature; galvanic cell measurements at high temperatures (1100-1400^{o}K); heat capacity measurements from 4-1300^{o}K; computer generated phase diagrams and thermodynamic functions.

453. MODELING OF ULTRASONIC NON-DESTRUCTIVE EVALUATION OF COLUMNAR STRUCTURES IN ANISOTROPIC MATERIALS — $ 98,500 — 01-5

B. R. Dewey - Dept. of Engineering Science and Mechanics
Phone: (615)-974-2487
B. F. Oliver - Dept. of Chemical, Metallurgical and Polymer Eng.
Phone: (615)-974-2420

Modeling of ultrasonic waves using finite element method; experimental ultrasonic measurements on Inconel and nickel specimens; materials preparation of nickel single crystals and bicrystals; measurement of ultrasonic transmission/reflection at bicrystal boundaries; ultrasonic measurements to be used to provide data for the finite element solutions to wave propagation; frequency dependent attenuation in single crystals.

UNIVERSITY OF TEXAS

454. POLAR FLUIDS: PHOTOEMISSION AND ELECTRONIC ENERGY LEVELS — $105,000 — 02-2

J. C. Thompson - Dept. of Physics
Phone: (512)-471-5926
P. R. Antoniewicz - Dept. of Physics
Phone: (512)-471-3766

Measure photoinjected current in polar fluids (NH_3, H_2O and alcohols) as a function of bias, photon energy and temperature. Ag electrode illuminated by pulsed dye laser. Will measure i-V curves and determine electronic energy levels, interfacial work function. Concurrent theoretical work will include calculation of density of states.

UNIVERSITY OF UTAH

455. THE EFFECT OF PROCESSING CONDITIONS ON THE RELIABILITY OF CROSS-LINKED POLYETHYLENE CABLE INSULATION — $ 83,809 — 03-2

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

Studies of the internal structure of polyethylene insulation, including the effect of melting and recrystallization on the interfacial boundary between the insulation and the semiconducting layer. Morphology, dielectric loss spectra and treeing properties of an extensive series of miniature cables will be determined under carefully controlled extrusion, cross-linking and crystallization conditions. Apparatus for accelerated testing of "treeing" has been assembled and is being employed in studies of the aging process involving miniature extruded cables.

456. THEORETICAL AND EXPERIMENTAL STUDY OF SOLID PHASE MISCIBILITY GAPS IN III/V QUATERNARY ALLOYS — $ 45,587 — 01-3

G. B. Stringfellow - Depts. of Materials Science and Engineering and Electrical Engineering
Phone: (801)-581-8387

Miscibility gap studies in III-V quaternary alloys, including (1) development of models and techniques for calculating solid-solid miscibility gaps in quaternary alloys, (2) calculation of effects of coherency strain on the equilibrium phase diagram, (3) experimental determination of the miscibility gap in the system $Ga_xAl_{1-x}As_{1-y}Sb_y$ in both homogeneously nucleated platelets (without elastic strain) and liquid phase epitaxial layers on GaAs and InP substrates, and (4) miscibility study of $Ga_xAl_{1-x}As_{1-y}Sb_y$ alloys grown by the kinetically controlled organometallic vapor phase epitaxial technique. This includes the study, for nonequilibrium alloys, of spinodal decomposition and its effects on the electrical and optical properties of the alloys.

UNIVERSITY OF UTAH (continued)

457. ELECTROLYTIC DEGRADATION OF LITHIA-STABILIZED β" ALUMINA — $ 70,310 — 03-2
A. V. Virkar - Dept. of Materials Science and Engineering
Phone: (801)-581-5396

Studies of degradation of β-alumina near the melting point of Na, including effects of local enhancement of current density. Improvement of wetting characteristics of molten Na by addition of benign additives. The effect of grain size on degradation of β-alumina at room temperature.

VIRGINIA POLYTECHNIC INSTITUTE AND STATE UNIVERSITY

458. FRACTURE MECHANISMS IN GLASS-CRYSTAL COMPOSITES — $ 74,774 — 01-2
D. P. H. Hasselman - Dept. of Materials Engineering
Phone: (703)-961-5402

Fracture mechanisms in glass-crystal composites with a cordierite glass-ceramic and its original (non-crystallized) glass as the principal materials of study. Flaw introduction by micro-hardness indentation and crack characterization by scanning electron microscopy. Characterization of localized stress distribution near crystalline dispersions, sub-critical and critical crack propagation behavior, associated crack-crystalline interaction, and mechanisms which control the nature (size, geometry) of the fracture-initiating flaw. Biaxial flexure and double torsion strength characterizations. Environmental and loading conditions include ambient room air and inert environments, and variable loading rates to establish strain-rate sensitivity.

459. HYDROGEN EMBRITTLEMENT TESTING — $ 38,400 — 01-2
M. R. Louthan, Jr. - Dept. of Materials Engineering
Phone: (703)-961-6825

Evaluation of the effective H_2 fugacity in electrochemically-charged steels by comparison with gaseous permeation data; mechanical testing of carbon and low alloy steels charged either electrochemically or in gaseous H_2 up to 65 MPa; comparison of fracture behavior of specimens deformed during vs after H_2 charging.

UNIVERSITY OF VIRGINIA

460. SPECTROSCOPY OF SURFACE ADSORBED MOLECULES — $ 89,000 — 02-2

R. V. Coleman - Dept. of Physics
Phone: (804)-924-3781

Investigations of the properties of surfaces and interfaces containing molecular adsorbates using inelastic electron tunneling (IETS), photoemission (ESCA), and Auger spectroscopies. IETS spectra will be obtained for a number of combinations of oxide substrate and metal overlayer electrode to establish the nature of the chemical and electronic interactions between molecules and interface. ESCA and Auger studies will be made on the same systems to augment the IETS work. Studies of UV-induced damage to molecules and photocatalytic effects on semiconductor oxides.

461. MAGNETIC IMPURITIES IN SUPERCONDUCTORS — $ 63, 000 — 02-3

J. Ruvalds - Dept. of Physics
Phone: (804)-924-3782

Study the origin of the exceptionally strong indirect exchange interactions among magnetic impurities in layered compounds like $NbSe_2$ and in rare-earth compounds such as LaGd, and (La,Th) Ce_x which are known to exhibit unusual electrical and magnetic properties. Extend the theory to the phenomenon of reentrant superconductivity and calculate the influence of external magnetic fields and varying temperature on the electrical resistance, magnetic susceptibility and thermodynamic properties of these compounds.

WASHINGTON UNIVERSITY

462. MICROSCOPIC DETERMINATIONS OF LATTICE AND ELECTRONIC STRUCTURES OF SOLIDS — $200,000 (2 years) — 02-2

P. C. Gibbons - Dept. of Physics
Phone: (314)-889-6271

A high-flux imaging, electron energy loss spectrometer will be used for microscopic determinations of electronic excitations and atomic structure in a wide range of metallic and semiconducting materials.

UNIVERSITY OF WASHINGTON

463. NUCLEAR MAGNETIC RESONANCE STUDIES OF ION MOTION IN SOLID ELECTROLYTES — $ 66,000 — 01-3
J. L. Bjorkstam - Dept. of Electrical Engineering
Phone: (206)-543-2177

Nuclear magnetic resonance (NMR) studies of spin-spin and spin-lattice relaxation times, effects of motion and structure upon the dielectric quadrupole NMR spectrum, and direct NMR diffusion measurements to study the solid electrolytes mixed•cation β-alumina and alkali containing borate glasses. Correlative studies involve electrical conductivity and thermal analysis. Temperature and frequency dependence of the spin-lattice relaxation to understand ion-ion and ion-lattice interactions and predict electrolyte systems with optimized conductivity. Other techniques invoked include gravimetric analysis, neutron activation analysis, X-ray diffraction, infrared absorption, thermomodulated uv-reflectivity, thermoelectric currents, and correlated light scattering.

464. RUBBER ELASTICITY — $ 56,000 — 03-1
B. E. Eichinger - Dept. of Chemistry
Phone: (206)-543-1653

Experimental studies of the elastic contribution to the chemical potential of a swelling agent in crosslinked and uncrosslinked polydimethylsiloxane. Theoretical studies on eignevalue spectra of Kirchoff matrices which describe random networks.

UNIVERSITY OF WISCONSIN, MADISON

465. MICROSTRUCTURAL ANALYSIS OF ION-CONTAINING POLYMERS — $ 79,000 — 03-1
S. L. Cooper - Dept. of Chemical Engineering
Phone: (608)-262-3641 or -1092

Studies of microstructure of several ionomer systems by EXAFS and Mössbauer spectroscopy. Investigations of relationships between composition and preparation variables and morphology and transport properties.

466. PREDICTION OF THE BEHAVIOR OF STRUCTURAL MATERIALS UNDER IRRADIATION THROUGH MODELLING OF THE MICROSTRUCTURE — $ 36,400 — 01-4
W. G. Wolfer - Dept. of Nuclear Engineering
Phone: (608)-263-6818

Modelling irradiation-induced void and dislocation loop nucleation and growth as stochastic clustering processes; effect of sink capture efficiency on forming vacancy type dislocation loops in metals, and extension to vacancy loop growth in Zr; equation of state for He in irradiation-induced voids and the role of He pressure on blister formation during irradiation; solute diffusion effects on void nucleation.

UNIVERSITY OF WISCONSIN, MILWAUKEE

467. INTERACTION OF LOW ENERGY ELECTRONS WITH SURFACE LATTICE VIBRATIONS — $ 57,117 — 02-2

S. Y. Tong - Dept. of Physics
Phone: (414)-963-4474

Theory of inelastic scattering of electrons by vibrating atoms and molecules at solid surfaces. Role of image potential in electron energy-loss spectroscopy (EELS) with low impact energies. Applications to H on W, and NH_3 and and CO on Ni, Pt, Rh, and Ir. Theory of lattice dynamics of clean and adsorbate-covered surfaces and of thermal diffuse scattering of electrons from clean transition metal surfaces. This program is strongly coupled with that of D. L. Mills, University of California/ Irvine.

SECTION C

Summary of Funding Levels

The summary funding levels for various research categories were determined from the index listing in Section D and estimating the percentage from the project devoted to a particular subject. There is overlap in the figures. For instance, funding for a project in diffusion in oxides at high pressure would appear in all three categories of diffusion, oxides, and high pressure.

During the fiscal year ending September 30, 1981, the Materials Sciences total support level amounted to about $87.5 million in operating funds (budget outlays) and $7.1 million in equipment funds. The equipment funds are expended primarily at Laboratories and are not shown in this analysis. Equipment funds for the Contract Research projects are included in the total contract dollars, being part of the operating budget. The following analysis of costs is concerned only with operating funds.

1. By Region of the Country:

		Contract Research (% by $)	Total Program (% by $)
(a)	Northeast ..... (Mass., Penn., N.Y., N.J., Del., D.C., Md., Vt., Conn., Me., N.H., R.I.)	46.9	21.0
(b)	South ..... (Fla., N.C., Tenn., Va., La., Ga., Ky.)	7.3	21.3
(c)	Midwest ..... (Ohio, Ill., Wisc., Mich., Mo., Minn., Ind., Iowa, Kan.)	24.0	36.6
(d)	West ..... (Ariz., Okla., Wash., Texas, N. Mex., Calif., Utah, Colo., Idaho)	21.8	21.1
		100.0	100.0

2. By Academic Department or Laboratory Division:

		Contract Research (% by $)	Total Program (% by $)
(a)	Metallurgy, Materials Science, Ceramics (Office Budget Activity Numbers 01-)	63.4	43.7

	Contract Research (% by $)	Total Program (% by $)
(b) Physics, Solid State Science, Solid State Physics (Office Budget Activity Numbers 02-)	29.0	42.9
(c) Chemistry, Chemical Eng. (Office Budget Activity Numbers 03-)	7.6	13.4
	100.0	100.0

3. By University, DOE Laboratory, and Industry:

	Total Program (% by $)
(a) University Programs (including those laboratories where graduate students are involved in research to a large extent, e.g., LBL, Ames)	37.5
(b) DOE Laboratory Programs	61.9
(c) Industry	0.6
	100.0

8.7
1.4
34.8

4. By Laboratory:

94.6

	Total Program (%)
Ames Laboratory	7.32
Argonne National Laboratory	20.55
Brookhaven National Laboratory	12.57
Idaho National Engineering Laboratory	0.54
Illinois, University of (Materials Research Laboratory)	3.02
Lawrence Berkeley Laboratory	6.78
Lawrence Livermore National Laboratory	1.36
Los Alamos National Laboratory	3.03
Mound Laboratory	0.29
Oak Ridge National Laboratory	19.84
Pacific Northwest Laboratory	2.15
Sandia National Laboratories	3.02
Solar Energy Research Institute	0.30
Contract Research	19.23
	100.00

17.6

5. By Selected Areas of Research:

	Number of Projects (Total=400) (%)	Total Program $ (%)
(a) Materials		
Polymers	5.0	1.9
Ceramics	28.8	15.2
Semiconductors	14.0	8.6
Hydrides	9.5	6.1
Ferrous Metals	20.8	12.2
(b) Technique		
Neutron Scattering	7.8	17.3
Theory	23.2	11.1
(c) Phenomena		
Catalysis	9.5	6.4
Corrosion	10.8	8.8
Diffusion	22.2	9.2
Superconductivity	11.0	6.9
Strength	19.5	9.4
(d) Environment		
Radiation	15.3	14.7
Sulphur-Containing	5.8	3.8

SERI
C.R. program
NBS program

SECTION D

Index of Investigators,
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Glass

20 214
38 216
42 218
44 222
68 310
80 322
107 326
130 339
132 390
156 419
157 436
158 458
463

Nitrides

105 339
123 353
124 371
130 379
162 383
303 394
325 440

Oxides

8 126 229 379
9 130 230 389
12 132 232 391
13 134 302 392
19 136 303 394
33 137 310 397
35 138 312 400
38 139 324 403
41 150 325 407
44 153 329 411
54 160 334 415
68 162 340 417
78 171 353 425
79 180 365 428
83 206 370 430
86 214 371 431
87 216 372 438
106 217 374 442
108 218 376 460
123 219 377 463
124 225

Composites

1 189
22 199
23 200
27 201
56 338
72 343
88 344
111 358
132 363
135 458
183

Fast Ion Conductors

33 202
53 204
61 318
68 326
80 329
106 393
110 401
111 407
118 420
184 424
187 432
189 457
193 463
195

Graphite, Carbon, and Coal

31 201
34 202
37 207
81 211
100 307
121 357
122 359
135 360
149 361
154 362
172 414
184 421
199

Hydrides

6 67 183
11 69 184
12 73 188
16 79 193
21 87 197
22 101 199
25 109 201
26 111 319
32 116 356
39 117 361
42 121 381
58 164 397
64 174

Intermetallic Compounds

11	40	73	184	215
17	42	75	188	325
18	43	77	189	342
23	46	81	190	349
24	47	83	191	359
25	52	128	193	363
26	53	143	195	378
27	61	145	198	387
32	64	147	199	397
36	67	149	201	409
38	69	153	206	446
39	72	183		

Ionic Crystals

8	86	183	195
12	138	184	200
13	142	185	216
19	147	187	229
77	149	189	376
78	156	193	439
81	158		

Liquids & Amorphous Metals

15	80	149	199	222
31	87	161	201	308
52	88	168	202	315
54	95	178	204	328
59	111	184	207	345
67	122	190	209	354
71	141	193	210	399
77	147	195	215	444

Metals

Alkali

11	199
67	328
69	359
148	424
149	432
168	

BCC Refractory

1	33	99	122	189	215
2	39	101	123	191	323
5	42	106	124	193	341
6	46	109	145	194	357
11	47	112	149	195	404
16	67	117	153	197	411
21	73	118	177	198	
27	87	121	188	199	

Metals (Continued)

Ferrous

1	70	176	220	351	408
2	81	179	221	354	410
3	122	181	222	364	412
4	123	183	230	368	416
6	124	184	305	375	422
7	131	189	321	377	426
9	136	191	323	385	428
10	139	193	328	388	438
14	145	194	330	391	441
17	149	195	335	398	445
34	153	199	337	399	448
51	155	212	340	402	459
66	173	213	345	404	466
67	175	217	348	405	

MHD Materials

12	186
83	189
108	195
185	324

Polymers

33	207	344	407
97	225	350	439
111	229	352	455
184	309	358	464
194	338	388	465

Rare Earth Metals and Compounds

2	21	64	149	200
3	32	68	163	201
5	37	69	183	203
8	38	77	184	216
10	42	79	189	316
12	43	110	193	356
13	52	123	198	395
18	53	145	199	461
19	58	147		

Semiconductors

3	129	198	341
22	130	199	355
24	140	208	366
25	142	209	386
59	143	210	389
61	145	220	403
68	146	222	406
71	150	224	413
81	151	225	438
88	158	227	447
96	189	229	456
112	190	304	457
113	193	306	460
122	195	333	462

Acoustic Emission

6 346
68 341
130

Auger Electron Spectroscopy

14	132	199	230	406
15	139	208	232	412
37	151	209	233	447
40	152	211	334	449
47	153	212	345	450
69	158	213	367	460
73	175	214	377	
87	193	218	386	
128	198	225	394	

Computer Simulation

17	68	144	191	212	367	449
20	85	146	193	228	369	452
35	86	148	195	310	390	464
41	127	157	197	318	401	
44	128	161	198	326	423	
47	130	168	199	355	430	
61	139	190	204	360	448	

Elastic Constants

12	119	346
17	128	362
72	131	457
111	149	464
117	197	

Electron Microscopy

6	76	129	161	199	220	336	383	426
7	84	130	162	201	222	340	385	438
10	95	131	171	204	226	341	389	440
19	98	132	172	211	233	348	391	445
41	107	133	174	212	302	350	402	447
42	122	134	179	213	310	356	403	448
44	123	137	180	214	315	365	405	451
46	124	139	185	215	323	369	409	458
47	125	148	188	216	324	372	410	462
48	126	151	190	217	325	377	411	465
51	127	152	191	218	333	380	412	
69	128	160	195	219	334	381	422	

Electron Spin Resonance

22	110	200
25	142	222
26	185	318
54	189	400
57	190	

Field Emission and Ion Microscopy

37	341
42	391
123	416
225	418
226	429

High Temperature Heat Capacity

149
452

Infrared Spectroscopy

22	159	219	392
59	185	222	394
65	186	233	400
91	187	306	401
140	190	349	407
142	199	350	419
151	210	361	455
156	214	387	463

Internal Friction

2	117
6	130
20	197
41	308
75	329
100	352
101	

Ion Channeling, Scattering and Implantation

41	188	205
47	190	222
51	193	232
84	195	233
99	197	378
129	198	397
171	199	437
186	200	

Laser Beam Scattering

57	187	199	313	421
99	188	216	319	429
114	190	218	321	
141	193	228	382	
143	195	230	393	
152	198	232	401	

Low Temperature Specific Heat

3	178
18	307
26	308
38	316
55	386
111	387
147	452

Magnetic Susceptibility

18	58	203
25	64	343
38	142	345
43	183	356
55	188	446
56	193	461

Neutron Scattering

21	63	81	183	202
26	64	83	184	329
39	77	119	187	357
42	78	121	188	373
49	79	164	189	401
52	80	175	193	405
53				

Nuclear Magnetic Resonance

22	57	318
25	97	407
26	109	420
38	120	421
43	154	432
44	307	463

Optical Spectroscopy

23	115	186	216	400
24	141	187	218	406
59	142	190	224	407
66	143	193	227	413
69	156	200	230	419
86	157	205	232	421
91	159	208	361	447
113	185	210	392	463
114				

Positron Annihilation

42	141
75	215
82	308
86	

Sputtering

42	144	213
47	193	217
56	199	219
69	201	233
96	209	353
130	210	447

Synchrotron Radiation

24	87	199	397
39	112	202	398
57	113	229	399
64	173	329	428
73	192	334	450
81	195	354	465
83	198	396	

Theory

20	124	183	212	344	380	441
28	125	184	215	350	385	446
29	127	187	225	352	390	448
30	128	188	304	354	400	453
38	130	190	305	355	401	454
42	131	191	309	359	404	456
44	133	192	314	360	405	457
59	142	193	320	366	409	461
61	145	195	322	367	413	463
67	146	198	326	368	414	464
72	149	199	327	369	430	465
85	167	202	329	373	432	466
91	168	204	338	375	438	467
113	170					

Thermal Conductivity

111	177	317
128	189	343
159	200	387
160	207	455

Thermodynamics

11	78	149	310	427
25	91	155	317	430
36	119	166	322	438
44	130	168	359	440
58	132	203	360	452
59	133	204	376	456
66	136	206	386	457
67	142	307	415	461
68	147	309	419	

X-Ray Photoelectron Spectroscopy

14	87	395
23	112	396
24	198	398
32	211	403
38	213	421
40	214	450
68	233	460
81	374	
84	384	

X-Ray Scattering

14	56	187	219	394
15	64	189	308	396
17	81	190	319	398
24	83	192	340	399
25	107	195	345	400
26	119	199	347	402
27	121	201	350	421
31	123	202	354	424
38	127	210	357	427
39	130	215	361	428
42	160	216	378	455
44	173	217	383	463
53	186	218	389	465

Catalysis

31	66	140	209	396	444
33	69	145	225	399	451
37	74	153	227	402	460
40	87	193	233	403	
57	105	198	355	418	
61	110	199	374	426	
64	133	202	392	428	

Channeling

42	199
193	222
198	

Corrosion

14	92	139	203	230	377
50	93	150	205	232	388
51	104	152	209	233	399
66	132	155	213	313	410
67	134	176	214	330	411
70	136	199	222	334	425
90	137	200	227	351	427
					459

Crystal Structure, Atomic Distribution and Crystal Transformations

8	73	124	184	215	392
9	78	125	187	216	403
25	79	126	188	310	416
26	81	127	189	315	420
27	83	128	190	324	424
31	85	130	191	325	426
32	87	133	192	326	428
33	95	145	193	340	440
36	97	146	195	341	455
38	101	149	198	347	456
39	104	153	199	354	462
42	106	160	200	359	463
58	114	162	201	360	
65	119	164	202	374	
66	122	173	203	380	
72	123	183	209	390	

Diffusion

1	59	128	152	199	315	376	430
2	65	129	161	200	322	377	432
3	68	130	163	204	326	381	436
10	72	132	176	207	341	407	439
13	82	133	184	213	352	412	440
14	101	134	185	214	353	417	442
16	106	136	186	217	355	419	447
42	118	137	187	222	358	420	449
44	122	142	190	231	359	424	451
47	124	149	193	233	360	427	457
51	126	150	197	312	369	429	463
							465

Dislocations

6	111	142	191	331	404	451
41	117	161	193	333	406	466
42	122	162	195	335	412	
76	124	175	197	337	422	
85	126	179	199	348	428	
86	128	185	215	369	431	
102	129	186	315	380	438	
105	130	190	324	397	439	

Erosion

50	199	232
69	200	321
93	207	379
130	223	408
180	230	

Electron and Ion Conduction

9	64	184	204	392	413	456
13	68	185	209	393	420	463
42	83	187	318	399	424	465
44	85	190	326	401	432	
53	135	193	329	403	436	
59	148	194	359	406	442	
61	152	202	389	407	447	

Electronic Structure

11	39	82	143	184	210	437
12	40	85	145	186	225	454
15	42	87	146	190	231	457
18	61	112	147	193	354	462
24	66	116	149	198	355	
33	68	120	168	200	390	
36	69	122	170	208	398	
38	81	142	183	209	432	

Magnetism

15	40	61	127	184	461
18	43	64	142	193	
21	52	77	145	331	
25	55	79	147	345	
38	56	85	151	399	
39	58	120	183	450	

Materials Preparation and Characterization

5	64	112	187	209	312	391	440
15	67	115	188	210	336	392	442
19	68	128	189	211	339	394	447
22	69	130	190	213	342	400	455
23	71	132	191	214	347	402	456
25	72	133	194	217	352	403	457
26	83	137	195	218	356	406	458
31	87	139	196	219	359	407	465
33	88	141	198	220	360	413	
34	95	149	199	223	363	415	
35	96	151	200	228	365	419	
38	99	171	201	230	370	420	
40	100	183	203	232	371	421	
42	104	184	206	233	380	424	
44	105	185	207	303	383	431	
53	108	186	208	310	389	436	

Nondestructive Evaluation

7	167	199	405
12	182	200	441
20	184	233	453
130	187	346	
141	189	397	

Phonons

18	78	144	183	401
21	79	145	184	403
23	81	146	187	430
52	85	147	190	463
58	128	164	193	467
59	140	168	195	
61	143	170	314	

Photovoltaic and Photothermal Phenomena

3	96	190	210	391	454
22	113	193	233	392	456
24	115	199	304	406	
37	129	208	333	413	
71	151	209	356	447	

Point Defects

2	83	129	179	194	315	417
10	86	130	184	195	325	428
13	111	135	185	197	335	430
27	113	136	186	199	341	466
42	117	142	188	215	357	
44	119	143	190	216	401	
47	122	145	191	222	404	
54	124	161	192	224	412	
82	128	175	193	231	416	

Precipitation

3	107	186	200	365	456
19	122	188	231	370	
35	123	189	310	371	
39	124	190	315	380	
42	128	191	322	409	
44	129	192	325	412	
47	130	195	339	427	
98	149	199	360	430	

Recovery and Recrystallization

34	128	192	199	412
95	138	193	215	422
99	189	194	337	448
107	190	195	348	

Sintering

8	130	190	360	440
19	132	200	365	
98	133	201	372	
104	137	216	383	
108	149	312	409	

Solidification

1	190	201	393
85	192	307	430
91	193	319	
181	195	320	
189	199	360	

Strength/Fracture

6	102	160	211	305	344	379	412	457
9	104	162	212	321	346	383	436	458
20	123	175	218	323	358	385	438	459
76	128	191	223	328	363	404	445	
95	130	194	231	338	364	408	448	
99	137	200	303	342	368	411	449	

Strength/ Constitutive Equations

41	309	439
128	311	448
130	337	
162	364	

Strength/ Fatique

7	175	405	445
95	191	408	448
123	305	438	455
128	337	439	
131	385	441	

Strength/ Creep

6	128	215	337	405	442
8	130	305	339	422	443
41	137	309	364	431	448
95	175	311	365	438	449
104	191	336	368	439	466

Strength (Continued)

Flow Stress

6	123	207	335	342	380	448
10	128	303	336	344	381	459
41	139	323	337	348	385	466
102	162	324	338	358	404	
105	191	331	339	379	439	

Stress-Corrosion Cracking

7	150	381
32	199	388
76	205	410
130	212	
131	221	

Superconductivity

1	33	58	88	178	199	397
5	40	64	105	183	316	446
18	46	72	116	184	343	460
21	52	75	144	188	349	
22	53	77	145	189	363	
24	55	83	146	193	378	
27	56	85	147	194	387	

Surface Phenomena and Thin Films

14	85	153	219	386	465
19	87	158	222	388	467
22	88	164	225	391	
23	101	188	226	392	
24	112	190	229	394	
35	114	193	233	396	
37	115	195	307	398	
40	116	198	310	399	
42	120	199	314	413	
47	122	200	326	414	
57	126	201	334	415	
61	132	205	341	418	
66	139	208	355	419	
69	140	209	356	426	
71	141	210	366	427	
73	145	212	367	437	
74	146	213	369	447	
80	148	214	374	450	
82	151	217	382	451	
84	152	218	384	460	
		219			

Welding

328
375

Gas/Oxidizing

13	130	153	230	377
44	132	185	232	392
48	136	189	233	411
51	139	199	302	425
92	149	200	360	432
123	151	213	367	442
124				

Gas/Hydrogen

7	73	153	197	312	397
11	101	162	199	313	398
16	124	163	210	323	412
32	126	165	212	335	416
42	131	166	222	346	425
48	132	185	229	356	432
58	134	191	231	381	442
69	149	193	305	388	459
71	150				

Gas/Sulphur-Containing

7	139	213	360
36	149	230	377
51	153	232	411
65	155	233	425
92	176	313	426
136	212	330	

Magnetic Field

23	75	194
38	142	200
57	147	304
58	183	316
64	184	366
72	188	446

Pressure Above Atmospheric

25	118	184	319
52	147	189	339
58	153	199	352
78	165	207	412
97	168	233	431
114			

Radiation/Electron

47	191	310
48	193	325
50	198	345
86	200	400
122	215	409
190	231	

Radiation/Ion

42	129	188	197	216
47	150	190	198	310
48	160	193	199	341
54	161	195	200	345
69	179	196	215	409

Radiation/Neutron

10	59	184	197
46	75	188	215
49	141	190	341
50	179	193	400
52	183	194	

Radiation/Photons

57	146	190	199	219
86	151	192	208	233
140	158	193	209	400
142	185	195	210	
143	187	198	218	

Radiation/Theory

47	190	231
50	193	466
179	215	

Radiation/Gamma

54	194
58	200
86	

Temperature

Very Low Temperatures

42	75	145	191	207
46	80	147	193	307
55	128	183	194	317
56	140	184	197	386
58	142	188	199	452
72	144			

High Temperatures

1	34	97	149	185	200	347
2	36	105	150	186	201	359
3	41	124	159	187	202	360
8	42	126	168	189	203	392
10	44	129	171	190	204	393
11	59	130	175	191	206	420
12	67	132	176	192	207	426
13	68	133	177	193	213	432
19	87	136	181	197	230	452
21	91	137	183	198	232	457
32	95	139	184	199	324	

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FY 1983 Congressional Budget
Program Title: Basic Energy Sciences
Organization: Office of Basic Energy Sciences, O.E.R.
Program Manager: Richard Kropschot
Fact Sheet Title: Material Sciences Summary

	FY 1981	FY 1982 (BA in Thousands)	FY 1983
Budget Summary			
Operating Expenses	89,083	96,194	108,700
Capital Equipment	7,100	7,960	8,510
Construction	300	600	3,000
Total	96,483	104,754	120,210

Budget Highlights

Full operational costs for the BNL-HFBR will be carried in FY 1983. The first full year of operational costs for NSLS and the LBL-HVEM will be borne in FY 1983. Research conducted at universities will be maintained, that at DOE laboratories will decrease considering cost-of-living, and research and operational costs associated with major facilities will increase. Research on theory, interfaces, ceramics and nuclear waste isolation will be emphasized, in addition to major facility related research, all at the expense of lower priority but still productive research.

Explanation of Budget Increases

Operating: +6.3M$ for operational costs and research associated with major facilities (e.g., 1.2M$ & 1.7M$ operational costs for NSLS and HFBR respectively)
+3.5M$ for universities on a base of 19.2M$
+2.6M$ for laboratory research on a base of 49.7M$
Capital Equipment: +.55M$ for NSLS primarily
Construction: 2.7M$ total for upgrading target area at WNR/PSR

Recent Accomplishments

Facilities:
. IPNS at ANL successfully built and began operation in FY 1982
. Highest voltage electron microscope in U.S. installed at LBL in FY 1982
. NSLS construction completed and will begin operation in FY 1982
. A User Materials Microanalysis Center was established at the University of Illinois

Research:
. Theoretical calculations completed showing that fundamental properties of solids can be predicted from the properties of constituent atoms alone, an important step along the way to enabling the design of new materials with prespecified properties.
. Development of a new process for the recovery of uranium from in-situ leach liquors that replaces the current batch process using ammonium hydroxide which had been virtually prohibited by EPA restrictions.
. A new method for fabricating a class of materials called intermetallic compounds which have excellent corrosion resistance for possible energy applications, but heretofore have seen limited use because of their brittleness.
. Development of a new class of dual phase steels containing few expensive alloying additions with potential for pipe line application.

ORNL

01- AEM [illegible]

02 - [illegible] micro program — [illegible] in 03 not happy

Capital [illegible]

phasing

High Temp [illegible]

LLL

D-T —

'83 glass · crystalline

01- theme —
battery —

14 MeV —

SERI

Polymer/Degradation

PNL tattered SD.

- Optical coatings

subcritical
coal microstructure
Davidson background
electron microscopist

Sandia/L

proposal

'82

'83 –

$600 eq

Sand/A

82

'83

SSP – 810 → 910

(personnel)

C-SCC –

Randich? – coatings

– Smyrl – –

Priorities – Glass Leaching

Corrosion

Shock Enhanced Reaction ?

Laser ?

21 [illegible] Layton X 0492

U of Illinois

Interdisciplinary —

Other Support —

Microanalysis Center —

✓ Jones —

Synthesis of Macrocyclics

Zangrilli

✓ Compound —

Don Keefer
583-8003

INEL

- Focus on Welding —
- NDE —
- Other proposals

LANL — - March 15 -

SSP —

'82 - ✓

'83 - ✓

Muon - low priority —
Far infrared —
Catalysis —
Synchrotron —
} low priority

Facility — personnel — equipment

Follow-on — not high priority

accomplish incl.
H/P. and theory in IVDE

LBL

Theory —

Yu - ? —

(other support) —

Hess - ?

Muller / Tobias — why not in same budget

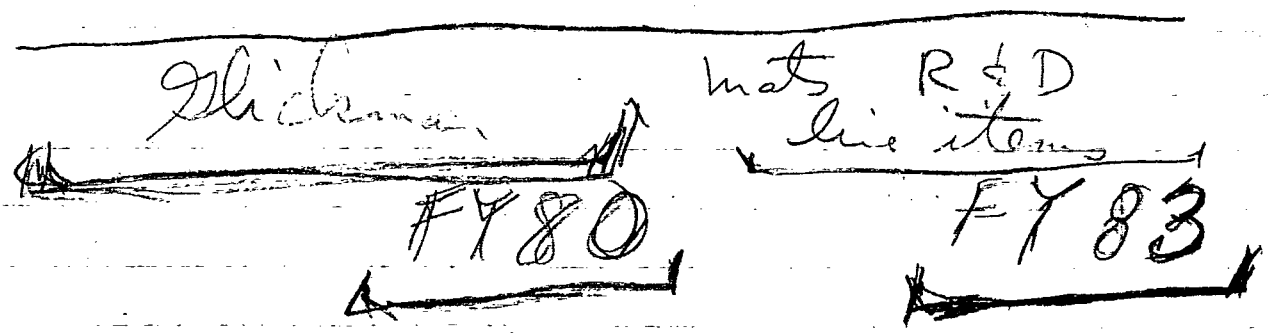
interdisciplinary

-01- EM — op research

Evans, Whittle — trading ?

J. Evans —

equip upstate


Mechanical
FY80
mats R&D
line items
FY83

Ames

budget category —
NDE —
restructuring —
ceramics processing —
Superconductivity —
Cryogenics —
strategic —
hiring people —

Finnemore —

01 — costs ? at NCR

H-storage
new mat } ?

Budget —

01 615 —

separate funding ?

[interdisciplinary]

BNL

Typo - '82 met.

Typo - '84 —

interdisciplinary

Amorphous mats —

electrochem ↘ ↗ other support?

Supercond?

H — Mortgage

SSP —

Rdmge in particle - Solid Int.
title's Rad Effects
Real Solids

Mats Synthesis —

NSLS — document 80%

HFBR — document 40% ARIM

ANL

MSD
IPNS —
Mech Prop. — direction
HVEM/Tandem — Research / Ops.
AEM / High Temp Corrosion

SSP
— electronic & magnetic why lumped?
SQUID — Biophysics
catalysts
→ good presentation

Chem — too general
Pulsed Neutron
— opposed to Synthesis —

Facility — < plus out
color photos

all involvement

— Industrial Involvement —

Materials Sciences

Categories of Research at Major Laboratories

	(M$) ANL	BNL	ORNL
1) Major Facility Related	7.25	9.26	3.30
2) Other Unique facilities, expertise, special equipment & apparatus	3.50	1.86	5.00
3) Close tie to other lab programs (applied) - i.e. underpin the technology effort	2.30	0.90	6.10
4) Multidisciplinary team effort on complex problem or one requiring many disciplines	4.65	2.00	3.20
5) Other, needed to complement lab efforts	0.80	0.40	1.20
	18.50	14.42	18.80

U.S. Department of Energy

ARGONNE NATIONAL LABORATORY

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Telephone 312/972- 4925

January 21, 1982

Dr. L. C. Ianniello, Director
Division of Materials Sciences
Mail Stop G256, GTN
U.S. Dept. of Energy
Washington, D.C. 20545

Dear Lou:

Enclosed is the Materials Science Division - Physical Research Program report "Erosion of Corroded Stainless Steel at Elevated Temperature". In this research Art Turner and Ken Natesan have studied the particle size, velocity, and angle of incidence dependence of erosion of corrosion product scales at high temperature. They have found that the erosion rate is at least an order of magnitude greater for the corrosion product scale than for the base stainless steel. The presence of sulfur in the corrosion environment leads to spalling of the scale at rather mild erosion conditions. Because of the importance of the synergism of combined corrosion and erosion for materials in a coal gasification environment, work is proceeding to establish the mechanism of the "ductile" erosive behavior of the normally brittle scales.

Best regards,

Frank

F. Y. Fradin
Associate Director
Materials Science Division

FYF:ph
encl.

xc: W. E. Massey
R. H. Bauer/DOE-CH
D. K. Stevens/DOE-WA
R. H. Kropschot/DOE-WA

ARGONNE NATIONAL LABORATORY

Materials Science Division Physical Research Program

Report for December 1981

Erosion of Corroded Stainless Steel at Elevated Temperature

(A. P. L. Turner and K. Natesan)

The processes of erosion and corrosion can be expected to interact synergistically. When a corrosive environment is present, the erosion process occurs in a surface layer whose chemical and mechanical properties have been altered by corrosion. This layer may be a surface passivating corrosion product scale, or it may be a region whose properties have been changed by penetration of elements from the environment. At the same time, the erosion affects the corrosion process by removing the corrosion product scales that would cause surface passivation. Thus erosion-corrosion may cause failure of a component under conditions where neither erosion nor corrosion alone would be serious.

One method of studying the complex process of erosion-corrosion is to separate it into several components that can be studied individually. The erosion behavior of scales preformed by exposure to a corrosive environment can be measured under non-corrosive conditions. The erosion resistance of the scales can then be correlated with their structure and composition and the conditions under which they were formed. This will help identify those properties of the corrosion product scales that are important to erosion resistance. In the present study, samples of Type 310 stainless steel were exposed for 60 hours at 750°C to multicomponent gaseous environments containing oxygen and sulfur as the active species. Four environments were initially chosen, as shown in the chemical equilibrium diagram in Fig. 1. All of the environments were such that thermodynamic equilibrium would dictate the

formation of oxide scales on Type 310 stainless steel. However, a previous study by Natesan[1] has shown that because of kinetic effects, the amount of sulfur in the scale increases with increasing sulfur potential. Thus the scales formed on the samples for this study have different compositions and structures. Unfortunately, the two highest partial pressures of sulfur resulted in scales that were too weak to withstand the thermal cycling required for the erosion tests at 500°C; these scales spalled from the substrates during a preliminary heat/cool cycle. The scales formed in the two most oxidizing environments were strong and adherent. They remained attached to the substrates after several temperature cycles between 20 and 500°C.

Erosion tests were carried out on the two latter sets of corroded samples. Weight loss of the samples was measured as a function of particle velocity, particle size, and angle of incidence. The eroded surfaces were examined by optical and scanning electron microscopy for evidence of the operating erosion mechanisms. All erosion tests were done at 500°C in vacuum.

Figure 2 shows the variation of the rate of erosion of the scales with particle velocity for 65-μm mean diameter SiC particles. Data are shown for incident angles of both 90° (Fig. 2a) and 20° (Fig. 2b). The erosion behavior of clean Type 310 stainless steel at 500°C is shown for comparison. The erosion rates are given as a dimensionless quantity, namely, mass lost by the sample divided by the mass of the incident abrasive. Tests were continued until the mass removed was equal to the estimated mass of the scale. The data show that the erosion rate of the scales was at least a factor of 10 greater

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[1]K. Natesan, "Corrosion and Mechanical Behavior of Materials for Coal Gasification Applications," Argonne National Laboratory Report ANL-80-5 (May 1980).

at 90° incidence, and a factor of 2 greater at 20° incidence, than the corresponding rate for stainless steel. For the measurements at normal incidence, there is a clear effect of sulfur in the scale; the scale formed in the gas mixture with lower sulfur potential is consistently the more erosion resistant. At glancing incidence this difference is much less apparent.

At normal incidence, the highest velocity, 81 m/s, caused rapid spalling of both types of scale. For the scale formed in the atmosphere with a higher sulfur potential, the erosion rate was such that more than half of the scale was removed after an exposure of only 4 mg/mm^2. The lower-sulfur scale was only slightly more durable. The critical velocity to cause spalling of the scale is dependent on both incident angle and particle size, because spalling was not observed at 81 m/s for either 65-μm-diameter particles at 20° incidence or 23-μm-diameter particles at normal incidence. A spalling criterion such as a critical particle momentum perpendicular to the surface would be consistent with these results.

Comparison of Figs. 2a and b shows that, in the absence of spalling, the rate of erosion is greater for 20° than for 90° incidence. This is somewhat surprising because rapid erosion at glancing incidence is usually associated with a micromachining or chipping mechanism that is characteristic of ductile metals. The chromium oxide scales might be expected to behave more like brittle ceramics, which erode more rapidly at 90° incidence. Such brittle erosion is associated with the propagation of subsurface cracks that leave a distinctive crater. The eroded sample surfaces were examined by optical and scanning electron microscopy and no brittle craters were observed. It is possible that this mechanism of material removal does not operate in the ~ 10-μm-thick scales studied here because cracks are too difficult to initiate

or propagate within such a thin layer. When the crack forms and propagates at the scale-substrate interface, spalling of the scale results. Figure 3 shows erosion rate measurements for two different abrasive particle sizes. The very slight particle size dependence is also characteristic of erosion of ductile materials. For brittle materials, the erosion rate usually increases as r^n, where r is particle radius and n is between 2 and 3.

These measurements demonstrate the presence of a substantial synergism between erosion and corrosion. Conversion of the metal substrate to an oxide scale reduces the erosion resistance by at least a factor of 10. Erosion above a critical intensity (where intensity is a function of particle velocity, size, and angle of incidence) causes spalling of the scale. Under these conditions, no passivating scale can survive on the material and corrosion will continuously take place at a rate characteristic of the bare metal. The high corrosion rate that would result may be accompanied by penetration of the grain boundaries by an aggressive species, leading to cracking. The presence of sulfur in the corrosion environment is found to degrade the erosion resistance of the scales on Type 310 stainless steel even when the sulfur activity is too low to have a major effect on the corrosion rate.

Future work will seek to establish more closely the correlation between the erosion resistance of the scale and its structure and properties. Microhardness and indentation fracture measurements can be used to establish the strength properties of the scales. Detailed SEM examination of eroded samples, including sections through the scale to reveal subsurface damage, will be performed to determine how the erosion mechanisms are related to the structure of the scale. The range of scale formation conditions studied will be extended by exposing samples to gas mixtures with higher sulfur content for

short times to form thinner scales. This should avoid the spalling that occurred during thermal cycling in some of the experiments.

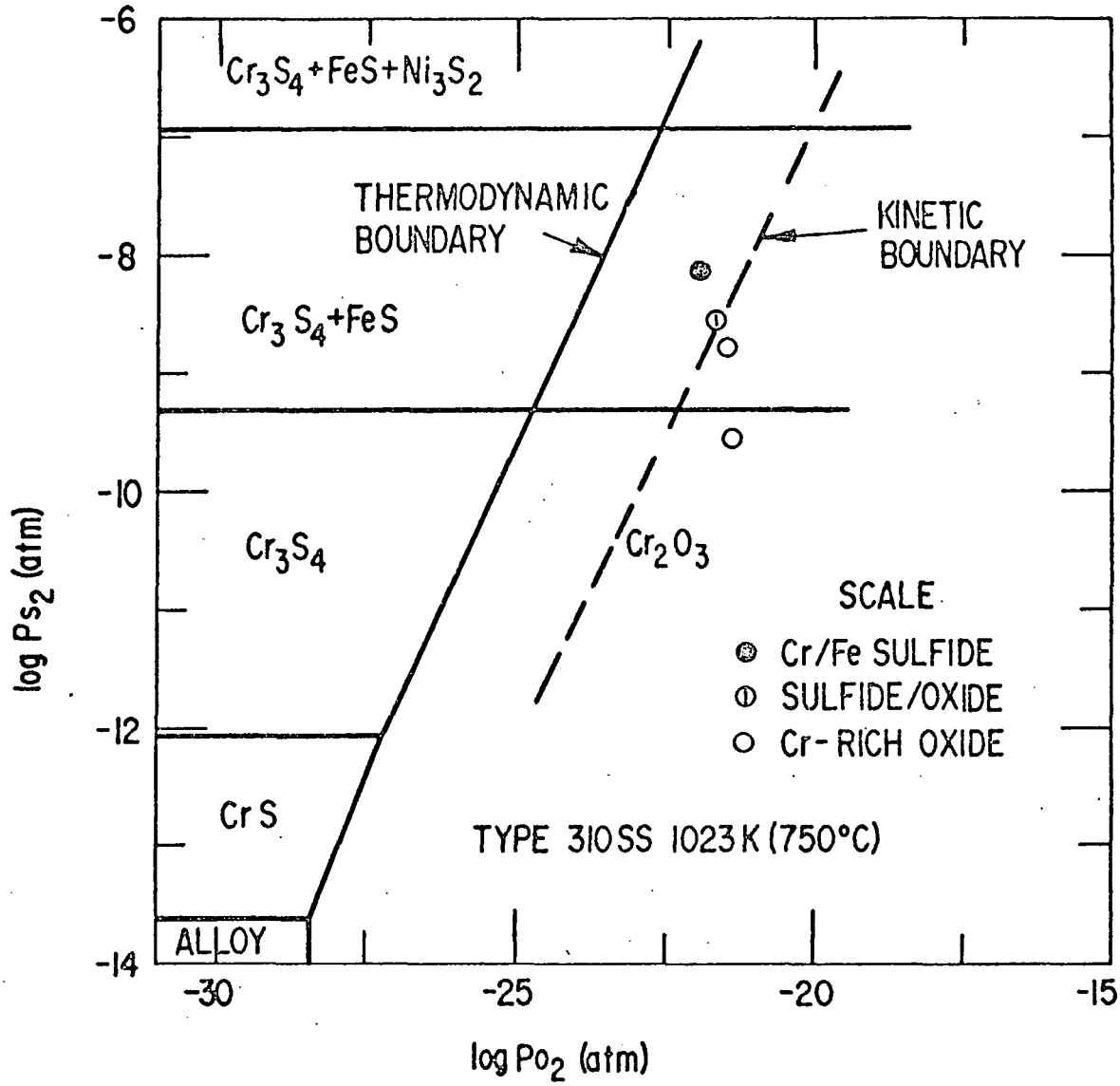

Fig. 1. Oxygen-sulfur thermochemical diagram for Type 310 stainless steel at 750°C. The four gas compositions to which samples were exposed in the present experiments are indicated by symbols, which also indicate the type of scale formed in each case. Only the scales formed in the two atmospheres with lower sulfur content were sufficiently adherent to withstand thermal cycling.

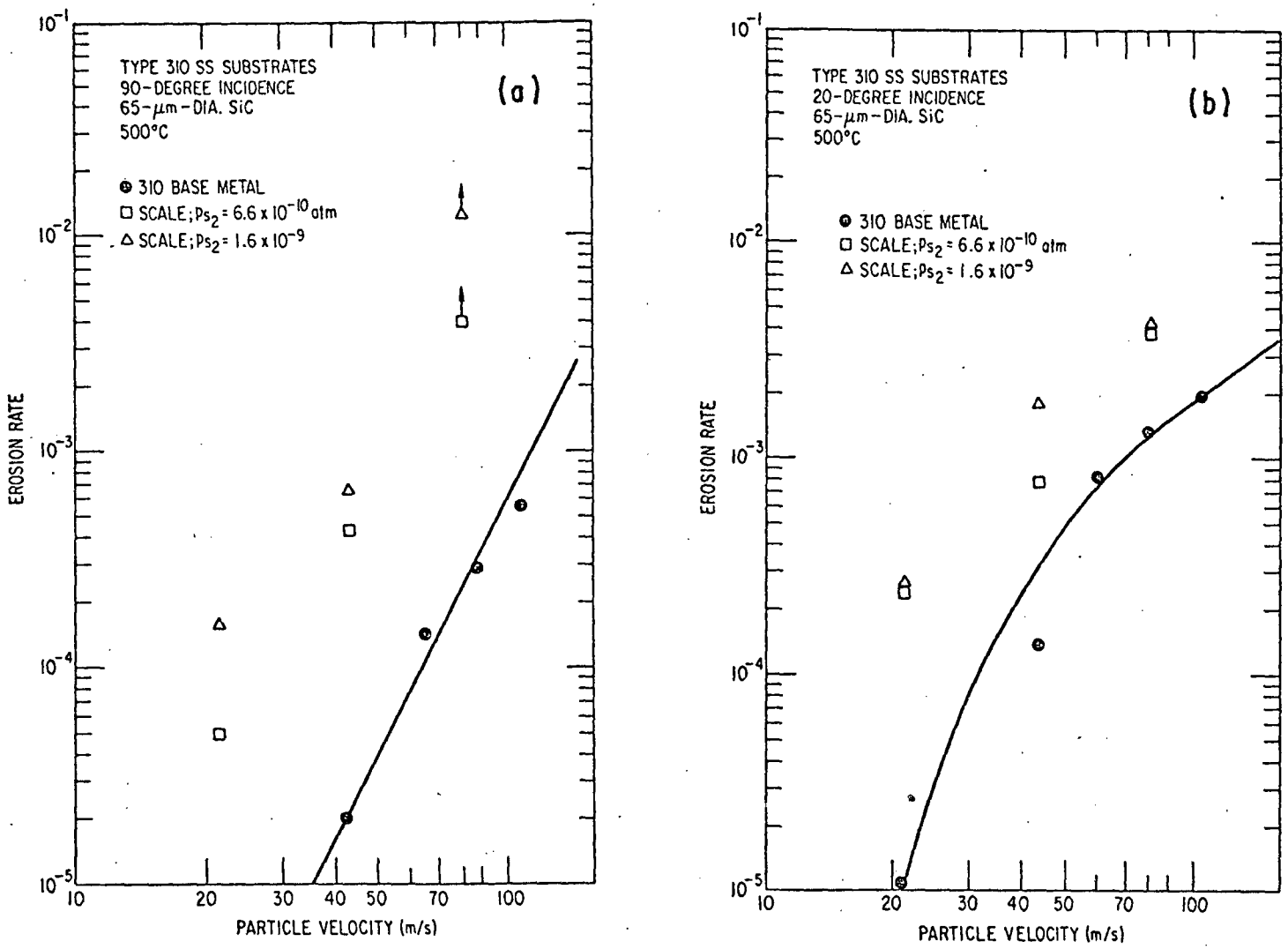

Fig. 2. Erosion rates of clean Type 310 stainless steel and two corrosion product scales formed on Type 310 stainless steel, eroded by 65-μm SiC particles incident at (a) 90° and (b) 20°.

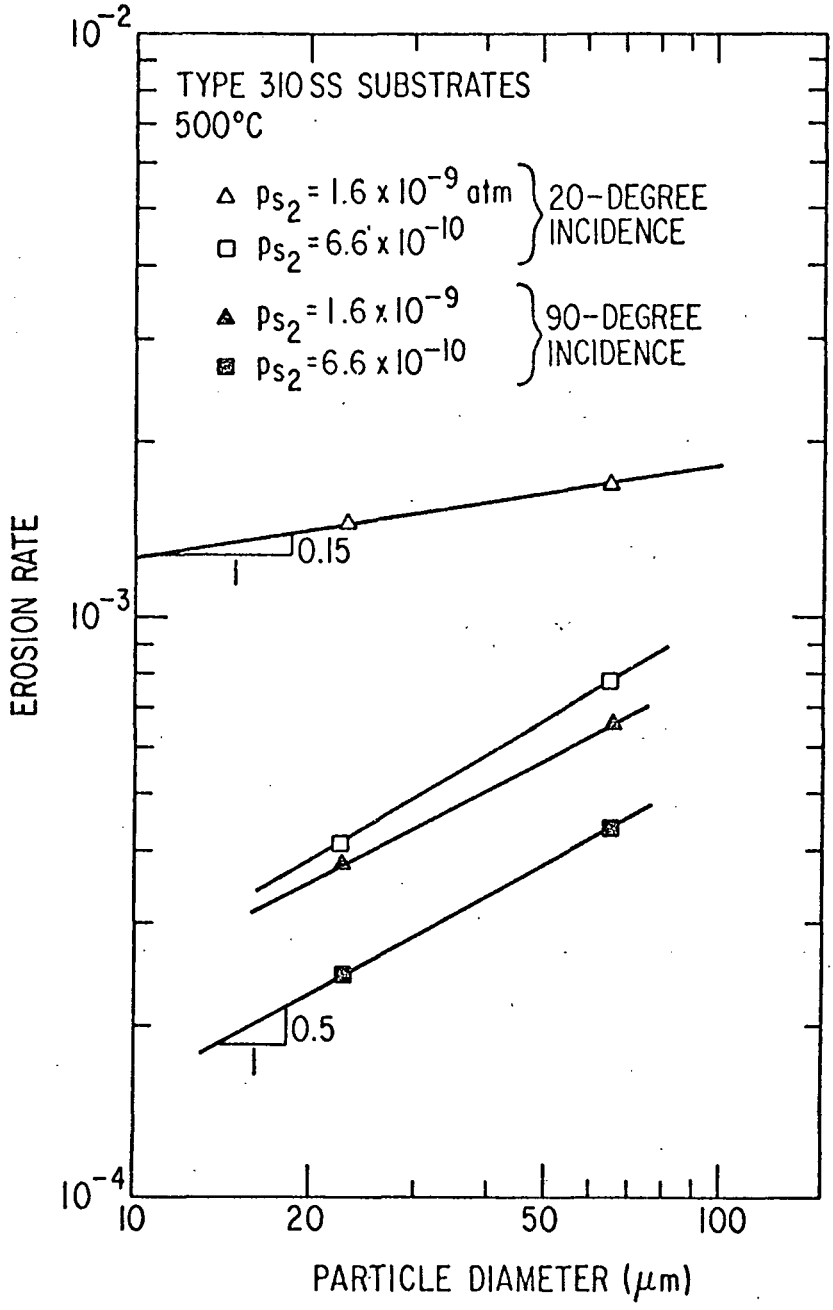

Fig. 3. Erosion rates of the corrosion product scales vs abrasive particle size.

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