TID-4005 (Pt. 1, 7th Ed.)

Summaries of the USAEC Basic Research Programs in Metallurgy, Solid State Physics and Ceramics

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(TID-4500, 25th Ed.)

SUMMARIES OF THE USAEC BASIC RESEARCH PROGRAMS IN METALLURGY, SOLID STATE PHYSICS AND CERAMICS

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INTRODUCTION

Under the authority and direction of the Atomic Energy Act, the Atomic Energy Commission supports and fosters basic research related to its overall program. Virtually all such research is performed by contractor organizations. Continuing programs are conducted in AEC-owned institutions operated by universities or industrial concerns. In addition, the Commission provides assistance to universities, other government laboratories, industrial laboratories, and others, who can contribute to the program of the Commission by research in their own laboratories.

While a certain amount of basic research is, of necessity, performed in association with projects with applied objectives, the central effort of the Commission in the support of basic research in the physical sciences is the responsibility of the Division of Research. Under its auspices, research is being supported in the fields of high and low energy physics, chemistry, materials science, and controlled thermonuclear processes. This document summarizes the program on materials science supported by the Office of Metallurgy and Materials Programs of the Division of Research.

The objective of the Metallurgy and Materials Programs is to insure that research is conducted which advances the body of fundamental knowledge used to cope with the broad spectrum of materials problems facing nuclear technology. The approach taken is to investigate material structures, properties, and phenomena in the most rigorous possible fashion so that they may be explained and predicted in terms of fundamental laws of nature. This program embraces the traditional disciplines of physical metallurgy, ceramics, crystallography, corrosion, etc., but each in its most basic context. The newer discipline of solid state physics occupies a position of major importance in the program. Special importance is placed on understanding in detail the effects of irradiation on materials and the methods and tools of all these disciplines are applied to this problem.

In terms of the distribution of funds, about two-thirds of the Metallurgy and Materials Programs are conducted in the AEC laboratories and, of the remaining one-third, most is spent in colleges and universities. At the end of the past fiscal year, June 30, 1963, the Office of the Metallurgy and Materials Programs was supporting 160 contracts in its contract research program, of which 142 were in 71 educational institutions.

Much of the research conducted at the AEC laboratories requires experimental and support facilities not found elsewhere, such as high flux reactors and facilities for handling highly radioactive materials. Also, at the AEC laboratories concentrated efforts by relatively large numbers of mature scientists of many disciplines may be devoted to specific problem areas for extended periods of time, such as pure materials preparation and characterization.

The offsite contract research program provides breadth and flexibility to the AEC program. By supporting such programs in universities, the AEC obtains the benefit of research conducted by those individuals who prefer an academic environment. For the most part, the offsite program is composed of small, short term projects in which graduate student participation is an important factor. The contracts supporting these projects originate from unsolicited proposals based on the scientific interest of the principal investigator. Of the many such proposals submitted to the AEC, those chosen for funding are selected on the basis of their scientific merit and their pertinence to the AEC program. The resulting contracts usually cover a one year period but may be renewed if the research continues to be productive and of AEC interest and if sufficient funds are available.

This report contains summaries of the research programs active during Fiscal Year 1963. Part I presents the research conducted in the AEC laboratories and Part II, the research conducted elsewhere. For the most part, these summaries were written by the investigators themselves. However, some editing has been done for the sake of consistency. The summaries have been indexed in terms of senior technical people involved and in terms of scientific content.

PART I

RESEARCH IN AEC LABORATORIES

Contractor: Ames Laboratory, Iowa State University, Ames, Iowa

Contract Number: W-7405-ENG-82

Present Contract Term: July 1, 1962 through June 30, 1963

Cost to AEC: $660,000

Contract Title: Basic Research in the Metallurgy Division

Investigators: F. H. Spedding, O. N. Carlson and staff

Scope of Work: A. Preparation and Properties of Pure Materials

1. Preparation of Pure Metals and Metal Compounds
O. N. Carlson, R. E. McCarley, D. T. Peterson, J. Verhoeven and H. A. Wilhelm

Work on the treatment of cesium and rhenium bearing ores or concentrates was begun with the objective of preparing these metals and their compounds in very high purity. The chemical properties of the halides of Nb, Ta, W, Mo and V are under investigation since these compounds are of interest to the preparation and/or purification of these metals. The tetrachlorides and tetrabromides of Nb, Ta, W and Mo were shown to be isostructural. The vaporization reactions and the nature of the vapor species are being determined and the nature of solid solutions of mixed halides investigated.

The preparation and purification of the less common metals continued using various methods of reducing high purity compounds followed by refining processes such as electron beam melting, iodide refining, distillation, selective deoxidation, electron beam- and arc-zone refining. Thorium metal has been purified by electron beam zone refining with significant reductions in the carbon and nitrogen contents. Iodide vanadium has been given further purification by electron beam melting and new techniques for reducing high purity V_2O_5 are being studied. The aluminum reduction of Nb_2O_5 with subsequent electron beam melting shows promise as a new method of producing high purity niobium. Increased emphasis will be given to preparing high purity rhenium metal.

A new program is being initiated under Dr. John Verhoeven on studying the effect of an electric field on the transport of solute impurities during zone refining. Correlation with present theories will be attempted.

2. Elastic Properties

J. F. Smith

A program for the determination of elastic constants of single crystalline metals has been in progress for several years because of the fundamental importance of these constants to theories of lattice dynamics, metallic bonding and mechanical properties. Extension of the use of ultrasonic techniques to the measurement of other properties is also planned. Single crystals of rhenium were grown and its elastic constants are being determined. Like wise the elastic constants of the three crystalline forms of thallium are being measured. Those for the hexagonal form have been completed and single crystals of the f.c.c. form grown using indium to stabilize this form. The thermal expansion of sodium-tungsten, bronze, and magnetic susceptibility of indium are in progress. Further measurement of elastic behavior of single crystals using diffuse x-ray techniques will be carried out due to the discrepancy in results obtained by the two methods.

3. Effect of Impurities on the Plastic Deformation of Metals

O. N. Carlson, D. T. Peterson and H. A. Wilhelm

A study of the effect of impurities upon the brittle-ductile transition and other mechanical properties of the b.c.c. metals is continuing. Nitrogen raises the ductility transition temperature of single crystalline chromium from -80°C for the iodide metal to +40°C for the 0.11 w/o N alloy. The maxima in the tensile strength associated with strain-aging are shifted from 300°C and 410°C in pure chromium to 410° and 510°C in chromium containing 150 ppm N_2. The role of nitrogen in strain aging and strain age hardening in chromium is being studied by tensile and electrical resistivity measurements and electron microscopic observations. This work will be extended to include the effect of quenching and solute size and distribution on the transition temperature and strain age hardening.

Similar studies on vanadium indicate that this metal is relatively insensitive to embrittlement by nitrogen and carbon and no strain aging effect that can be directly attributed to these impurities has been found. Further purification with respect to carbon is required before the effect of this impurity on vanadium can be ascertained.

The effect of strain rate, temperature and impurities on the plastic properties of thorium is being investigated. Thorium, which has a tensile yield point of 18,000 psi at room temperature has been observed to creep at an appreciable rate at stresses as low as 10,000 psi. The influence of alloying with carbon and cerium on the mechanical properties will be measured and the deformation of high purity single crystals will be investigated.

B. Properties of Alloys

1. Structure and Deformation Properties of Superlattices

F. X. Kayser

A program is being initiated on the deformation behavior of superlattices. Short range ordering in the Fe-Al system in the composition of the ordered phase Fe_3Al, and the yield point associated therewith will be studied. The defect structure and the domain structure of the ordered region will be studied employing various techniques including the use of transmission electron microscopy.

2. Structures and Thermodynamic Properties of Intermetallic Compounds

J. F. Smith, D. T. Peterson and P. Chiotti

Phase relationships and the thermodynamic properties of the intermediate phases are being studied for several different types of systems. The phases that exist in the metal-metal hydride systems of the alkaline earth and rare earth metals is of particular interest. The calcium-calcium hydride and strontium-strontium hydride systems were investigated. A phase transition was observed at 230°C in strontium metal containing hydrogen but not in the hydrogen-free metal. The structure of metal-carbon-hydrogen ternary compounds will be investigated employing x-ray diffraction, nuclear magnetic resonance and neutron diffraction techniques.

The thermodynamic properties of alloy phases plays an important role in the prediction of the products of metal reactions and in understanding the energetics of alloy phases. Thermodynamic properties are being measured by electromotive force, calorimetric or vapor pressure techniques for correlation of these properties with the structures in an attempt to evaluate the strength and directionality of the interatomic bonding of intermetallic compounds.

The structures of the two allotropic forms of YAl_3 were determined and those of Nb_2Sn_3, Nb_3Sn_2, Y_2Mg_5 and Y_3Mg_{17} are currently being investigated. The measurement of the magnetic susceptibility of a family of compounds with the fluorite structure is in progress. The elastic constants and enthalpy of formation of $CaMg_2$ were measured.

The phase diagrams for the zinc binary systems of thorium, zirconium and yttrium have been worked out and the structures and some thermodynamic properties of the intermetallic compounds in these systems were determined. A rigaku specific heat and differential thermal analysis apparatus is being used to measure the specific heat and heat of transformation of YZn_2. The specific heats of the other six compounds in the yttrium-zinc system will also be measured over the temperature range of 100 to 600°C. This work will be extended to include zinc compounds of uranium, thorium, zirconium and cerium.

The equilibrium vapor pressures of magnesium binary alloys have been determined for a number of systems from which the thermodynamic function may be computed. Work on the Th-Mg system has been completed and is well along on the Co-Mg system. Determination of activity by electromotive force measurements on vanadium-aluminum alloys is being attempted. Also a differential acid solution calorimeter has been designed and is being used in the determination of the enthalpies of formation of the aluminum-rich compounds of vanadium.

3. Properties of Metallic Solutions

D. T. Peterson, A. H. Daane and F. X. Kayser

The nature of metallic solutions, both liquid and solid, is being studied by several investigators. One program is directed toward the nature of metals and alloys using the rare-earth metals because of the unique similarity of their outer electronic structures. Such properties as vapor pressure, electrical resistivity, heat capacity, magnetic and phase equilibria are being investigated for several rare-earth alloy systems. A very interesting and significant observation was that of the existence of the samarium-type structure in solid solutions between light and heavy rare earths. A more detailed investigation of this phenomena is planned. The physical properties of scandium metal have been characterized and the use of scandium in alloying studies with other rare earths is now possible. The magnetic nature of YMn_4 has been studied and the magnetic properties of other rare-earth alloys will be investigated. The nature of bonding in rare earth borides has been tested and found compatible with proposed models.

A study of the nature of solid solutions employing high-precision methods for measuring density as a function of composition will be initiated. From these measurements the partial molar volumes of the solutions and other properties of thermodynamic interest will be obtained. The nature and valence state of a metal when it is dissolved in its halide salt is being determined by studying alkaline earth metals in their liquid halide salts. The vapor pressure of the metal over the solution is being measured and the diffusion of the metal solute in its liquid salt is being studied by observing the rates of evaporation of the metal from the solution. Vapor pressure data on calcium in solution in $CaCl_2$ indicate that two solute particles are formed for each calcium atom in solution. This work will be extended to strontium and barium chloride solutions and to solutions of the alkaline earth metals in their iodides and bromides.

The diffusion of the interstitial atoms, hydrogen, carbon, nitrogen and oxygen in thorium, zirconium and the rare-earth metals is being studied. The effect of non-metallic impurities on the physical and mechanical properties of a metal is related to the kinetics of the diffusion process. Study of the diffusion of hydrogen in barium, europium and ytterbium is currently underway and the diffusion of carbon in a selected group of metals will be measured to permit testing of several theories of interstitial atomic diffusion.

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M. E. Kirkpatrick, J. F. Smith and W. L. Larsen, Acta Cryst. 15, 894 (1962)

Contractor: Ames Laboratory, Iowa State University, Ames, Iowa

Contract Number: W-7405-ENG-82

Present Contract Term: July 1, 1962 through June 30, 1963

Cost to AEC: $965,000

Contract Title: Basic Research in the Solid State Division

Investigators: F. H. Spedding, D. J. Zaffarano and staff

Scope of Work:

1. Electronic Structure of Crystalline Solids
R. G. Barnes, G. C. Danielson, A. V. Gold, R. H. Good, J. M. Keller, Sam Legvold, A. R. Mackintosh, R. C. Young and D. J. Zaffarano

The details of the Fermi surfaces of pure metals are being investigated using the de Haas-van Alphen (Gold) and magnetoacoustic (Mackintosh) effects, angular correlation in positron annihilation (Mackintosh, Zaffarano), size effect (Young) and magnetoresistivity (Mackintosh) measurements and cyclotron resonance (Young). While the general emphasis is on the transition metals, the de Haas-van Alphen effect has been studied in lead for pulsed fields of up to 200 kilogauss, with results which correlate well with earlier models and which can be represented theoretically through the use of an orthogonalized plane wave model. This work is continuing on single crystals of tungsten, molybdenum and iron. In particular, this effect was seen for the first time in iron in single crystal iron whiskers. The data for iron can be interpreted in terms of an internal magnetic field in the iron which is several times the saturation value. Similar conclusions have been drawn from anomalous Hall effect measurements in ferromagnetics in the past, and Hall effect measurements are being made on similar iron whisker samples. The positron annihilation technique has been used to demonstrate the differences in the electronic structure of liquid and solid mercury. Measurements of this type are continuing with particular emphasis on those substances for which more conventional Fermi surface measurements are difficult or impossible.

Details of the electronic bonding in pure metals, alloys and intermetallic compounds are being studied by magnetic resonance techniques (Barnes). Typical problems involve a combination of high pressure and nuclear magnetic resonance techniques to study diffusion in lithium-magnesium alloys, and the investigation of the nuclear magnetic resonance of Y(89) in various intermetallic compounds of yttrium with Mn, Co, Ni, Fe and Cu. The details of the nuclear magnetic resonance in

pure indium have been mapped out experimentally and are being interpreted in terms of a theoretical model. Approximate formulas for energy levels needed in magnetic resonance work are being developed theoretically (Good). The anti-ferromagnetic transition in chromium is being studied as a function of the alloying of Cr with various first transition series metals using as detectors the nuclear resonance of cr(53) and a 1 percent tracer of vanadium, V(51). This transition, as well as a suspected similar transition in vanadium, also has been studied using thermoelectric power measurements (Mackintosh, Legvold).

2. Superconductivity

A. R. Mackintosh, F. H. Spedding and C. A. Swenson

The availability and experience of the Metallurgy Groups of the Laboratory make it natural that this program concern itself primarily with the superconductivity of the imperfectly understood transition metals and their alloys. The superconducting transitions in a magnetic field have been studied for both high purity tantalum and niobium (resistivity ratios about 2000) (Swenson). The behavior of these two related metals is basically different, with tantalum showing the "soft" superconducting properties of a classical type, while niobium transitions show what has been classified as "hard" superconducting behavior in the past. These experiments establish for the first time that it is possible for a pure metal, niobium in this case, to have as an intrinsic property a negative surface free energy between its normal and superconducting regions. High purity lutetium metal has been cooled to 0.27°K without exhibiting superconducting behavior, and the lanthanum-lutetium alloy system is being studied to investigate in the limit of small lanthanum concentrations the temperature at which lutetium is likely to become superconducting (Mackintosh, Spedding). Transition metal alloy systems are being studied systematically for superconducting behavior in metallurgically well-defined specimens (Swenson).

3. Thermodynamic Properties of Solids

G. C. Danielson, R. H. Good, D. E. Hudson, A. R. Mackintosh, J. M. Keller and C. A. Swenson

Measurements are being made of the thermodynamic properties of a number of different solids over a wide range of temperatures and pressures. Pulse heating techniques (Danielson) have been used to determine to 1400°K the heat capacity of zirconium, the thermal diffusivity of pure silicon, and both quantities for high purity Armco iron. The data for silicon in particular can be interpreted in terms of a lattice contribution and a large electron-hole recombination term. Mass spectrometric techniques (Hudson) are used in combination with a Knudsen cell approach to obtain the cohesive energies for both pure metals and intermetallic compounds. This work also has included basic studies of surface ionization and electron-ion collision cross-sections.

The contribution of anharmonic terms to the high temperature thermal expansion of solids has been calculated (Keller). The low tempera-

ture thermal expansions of aluminum, copper, sapphire and rubidium iodide have been determined down to 1.8°K using a mutual inductance variable transformer technique which has a sensitivity of 0.5 angstroms for the detection of sample motion (Swenson). This work, which basically involves lattice dynamics in one form or another, will be expanded to inelastic scattering experiments when the Ames Laboratory Reactor is completed (Mackintosh).

Pressure-volume-temperature measurements to 20,000 atmos. at temperatures from 20°K upwards have been obtained for solid xenon and for cesium metal (Swenson). These data show quantitatively the effects of temperature and pressure on the thermodynamic properties of the solids. A simple statistical theory of metals is being considered for the analysis of the alkali metal data (Good). The linear compressibility in 2000 atmos. pressure has been measured to 0.5 percent precision for various samples of copper and for single crystal silver (Swenson). These data show that a real difference exists between ultrasonic and bulk determinations of compressibilities, presumably due to dislocation contributions. The equation of state of solidified He^3 has been deduced from heat capacity measurements at temperatures down to 0.3°K and at pressure up to 2000 atmos. (Swenson). The anomalous properties of a thermodynamically-unlikely body-centered-cubic phase have been established.

4. Properties of Rare Earth Metals and Compounds
R. H. Good, J. M. Keller, Sam Legvold, A. R. Mackintosh and F. H. Spedding

The electrical transport and magnetic properties of rare earth metal single crystals are being studied experimentally in some detail (Legvold, Mackintosh, Spedding). Most recent work has been on terbium, holmium and gadolinium, with emphasis on thermoelectric power measurements. These data will be supplemented by both neutron diffraction and spin wave spectrum experiments with the Ames Reactor. Measurements of the magnetostriction constants of gadolinium and holmium single crystals also have been completed. The various available data for the rare earth metals have been analyzed (Mackintosh) to show the effects on the Fermi surfaces of the metals in the regions of magnetic ordering. In addition, the low temperature properties of terbium and dysprosium (magnetic and transport) were shown to be consistent with the hypothesis of an energy gap in the spin-wave spectrum. The magnetic properties of these metals are being studied theoretically on a phenomenological basis (Good, Keller). The optical absorption spectra of the rare earth ethyl sulphates are being determined experimentally (Spedding), and also are being calculated theoretically (Good, Spedding). Calorimetric determinations of the hyperfine interactions in rare earth metals and alloys are being undertaken (Spedding, Swenson),

5. Semiconductors and Compounds with Variable Stoichiometry
G. C. Danielson, Ronald Fuchs, D. E. Hudson, D. W. Lynch, J. M. Keller, A. R. Mackintosh and R. C. Young

The transport and thermodynamic properties of the series of semicon-

ducting compounds of the form Mg_2X (X = Si, Ge, Sn or Pb) are being studied extensively (Danielson). Present measurements include resistivity, Hall Effect, Seebeck coefficient, elastic constants, optical absorption and reflection coefficients (Lynch), photoconductivity, recombination radiation, and low temperature specific heat. Many of these measurements are being made over a range of temperatures and sample purities. Experiments to determine the effects of pressures of up to 13,000 atmos. on the resistivities have been initiated (Danielson, Lynch). An orthogonalized-plane-wave calculation of the electronic band structure of Mg_2Si is being undertaken (Keller). Work on other semiconductors includes the measurement of the microwave Hall effect in germanium (Danielson, Young), and the temperature dependence of the resistivity of diamond (Hudson).

Experiments on non-stoichiometric compounds of the sodium tungsten bronze type, Na_xWO_3 (where x can be varied from close to zero to close to unity), have been refined in an attempt to understand their electronic properties (Danielson). In particular, optical reflection (Lynch) and Seebeck coefficient data have been obtained for the sodium tungsten bronzes, as well as a more precise determination of the variation of lattice parameter with x. Two theoretical models (Fuchs, Mackintosh) have been proposed to explain not only the transport properties and various crystal structures of Na_xWO_3, but the properties of the other tungsten bronzes (such as Li_xWO_3).

6. Ionic Crystals and Color Centers
R. G. Barnes, Ronald Fuchs and D. W. Lynch

The properties of the color centers in CsBr are being investigated using both electron spin resonance (Barnes) and optical techniques (Lynch). The nature of the V_2 and V_3 centers which appear in the alkali halides also is being studied (Lynch). The luminescence of F centers in KCl is being studied as a function of pressure. The possibility of using a pseudopotential in theoretical investigations of color centers is being investigated (Fuchs). The theoretical aspects of the temperature and pressure dependence of the dielectric constant in ionic crystals also are being studied (Fuchs).

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Contract Title: PHYSICAL RESEARCH IN THE METALLURGY DIVISION

Investigators: H. H. Chiswik, Associate Director, Metallurgy Division

Scope of Work: A. Physical Metallurgy of Basic Reactor Materials
L. T. Lloyd

The objectives of the physical metallurgy studies are to provide basic data on the properties of reactor materials and to take advantage of their special structural properties in furthering the knowledge of certain problems in metal physics. The problems currently under investigation are:

1. Elastic Constant Studies
E. S. Fisher

Measurements of ultrasonic wave velocities in single crystals are being made to determine the nine fundamental elastic moduli over the entire temperature range of stability for alpha-uranium. Data are completed between 43° and 310°K, and some of the moduli have been measured below and above these temperatures, respectively. The work at low temperatures has revealed a transformation, other than crystal structure, at $42^{\circ} \pm 2^{\circ}$K. At elevated temperatures unusually large negative temperature coefficients were observed for some of the moduli upon approaching the phase transformation at 940°K. The studies are being continued.

Measurements for determining the elastic moduli in single crystals of alpha-zirconium have been completed between 4° and 1100°K. A large negative temperature coefficient was found for the shear modulus which corresponds to the proposed mechanism for transformation from h.c.p. to b.c.c. structure. A similar, but even greater, negative temperature coefficient was found for the same modulus in alpha-titanium. These results, together with those for alpha-uranium, suggest that there are fundamental correlations between unusually large temperature coefficients of elastic moduli and the occurrence of phase transformations. The measurements are being continued to complete the data over the entire temperature range of stability for alpha-titanium. Similar studies are being carried out with yttrium and iron above room temperature to explore the general applicability of this correlation.

2. Diffusion Studies

N. L. Peterson and S. J. Rothman

Diffusion of U^{235} in single crystals of alpha-uranium is being studied as a function of orientation. At 625°C the diffusion coefficients in the a and c directions are equal ($D = 1.94 \times 10^{-13}$ cm^2/sec), while that in the b direction is less than 10^{-14} cm^2/sec. The results are consistent with the relative jumb distances for diffusion in the crystal lattice. Further measurements are planned at other temperatures.

Impurity diffusion of Cr^{51}, Mn^{54}, Fe^{59}, Co^{60}, Ni^{63}, Cu^{64} and Nb^{95} have been measured in gamma-uranium. Niobium diffuses slower than self-diffusion while all the other diffuse faster. The results, when compared with the activation energy for self-diffusion, are in good agreement with the recent theory of LeClaire. The frequency factors and activation energies were low, ranging from $D_o = 2.7 \times 10^{-4}$ cm^2/sec and $Q = 11.9$ kcal/mole for Fe^{59} to $D_o = 4.6 \times 10^{-2}$ cm^2/sec and $Q = 39.4$ kcal/mole for Nb^{95}, and the arrhenius plots showed an upward curvature below 830°C. The measurements can best be explained by the vacancy mechanism, but the complete elimination of the interstitialcy mechanism is not possible at this time. A slight variation of either mechanism is necessary to explain the curved Arrhenius plots; the precise cause of the curvature is still open to question. The occurrence of a curved Arrhenius plot for self-diffusion is being investigated for other b.c.c. transition metals.

A study is in progress to determine the role played by magnetic order on atomic jump processes. Internal friction measurements of the Zener relaxation mechanism will be made in the ferromagnetic and paramagnetic states in several alloy systems. Also, quenched specimens will be used to determine the activation energy of vacancy motion in both magnetic states.

3. Magnetic Susceptibility Studies

D. J. Lam and D. O. Van Ostenburg

Studies of thermal expansion coefficients and elastic constants in single crystals of α-uranium have indicated unusual properties at low temperatures. A knowledge of the details of such anomalies is important for a better understanding of the electron structure in this metal.

The object of this work is to investigate the temperatue and crystallographic dependence of the magnetic susceptibility of single crystals of α-uranium, and to search for any anomaly below room temperature which can be related to the unusual behavior of the elastic constants and thermal expansion coefficients.

Preliminary results indicate that magnetic anisotropy exists below room temperature. Detailed studies are currently in progress.

4. Plutonium Physical Metallurgy

A. F. Berndt, M. B. Brodsky, L. Ianniello, L. T. Lloyd and M. Rosen

Techniques and equipment have been developed for preparing high-purity plutonium by electrolysis of impure anodes in a fused salt electrolyte. The work is continuing in order to provide a basic material in support of plutonium research programs.

A series of programs which are concerned with high purity alpha-plutonium are in progress. Because of radioactive decay, plutonium is subject to self-irradiation damage. The rates of defect production and their annealing characteristics are being studied by electrical resistivity and thermoelectric force measurements as functions of time at subroom temperatures. Also, the change of indentation hardness with time is being measured at temperatures between 25° and 120°C. Since visual observations of structure are important in physical metallurgy studies, attempts are being made to refine the metallographic techniques for alpha-plutonium. From considerations of the melting temperature and the temperature dependence of mechanical properties, it is feasible that plutonium may recrystallize within the alpha phase. This and grain growth characteristics are being studied for alpha-plutonium.

The ability to measure the physical properties of monoclinic alpha-plutonium as a function of crystal orientation is dependent upon the availability of single crystals. Several approaches to this problem are under investigation, among which are studies on the structure present in samples slowly cooled in a temperature gradient from the liquid state, and attempts to grow single crystals from solutions in liquid alkali metals at temperatures within the alpha-plutonium phase.

Since the properties of a metal are dependent upon prior metallurgical history, an investigation has been undertaken with the ultimate goal of characterizing the mechanism of the beta to alpha transformation in plutonium. Two types of experiments are in progress: 1) at-temperatue microscopy to observe surface effects upon phase transformation, and 2) ultrasonic measurements to determine the kinetics of transformation.

The unusual negative coefficient of thermal expansion for the f.c.c. delta phase of plutonium has been interpreted in terms of the electronic structure for this phase. Two investigations which relate to this problem are in progress. One approach deals with the effects of compostion and pressure upon the transformation temperature of delta-plutonium alloys. The second study concerns electron transport phenomena, such as electrical resistivity, thermoelectric force and Hall-coefficient, as functions of temperature and alloy composition. The latter measurements also are being made on the various other phases of high purity plutonium.

5. Plastic Deformation of Alpha-Zirconium Crystals

D. G. Westlake

The effects of hydrogen additions to single crystals of alpha-zirconium upon the deformation mechanisms are being investigated. Microscopic examinations have revealed that either slip or twinning can initiate microcracks in the brittle hydride phase during tensile tests at liquid nitrogen temperature. These microcracks

do not propagate catastrophically into the metalmatrix, but during continued deformation they grow slowly. Zone refining methods are providing material for preparation of single crystal specimens that will be used in an investigation of the effects of solute hydrogen concentration at subroom temperatures on the slip and twinning deformations.

B. Alloy Studies

1. Occurrence of Transition Element Intermediate Phases

A. T. Aldred, J. B. Darby, Jr., A. E. Dwight, D. J. Lam and M. V. Nevitt

The objective of this program is to isolate and study the factors which control the occurrence of intermediate phases in which at least one partner is a transition element. Knowledge of the controlling factors will make it possible to predict the existence of compounds in systems which are now unknown.

An exploratory survey has been made of the intermediate phases formed when Tc is alloyed with elements of the Sc, Ti, V, Cr, Mn and Fe groups. A total of 19 intermediate phases has been identified and found to be isomorphous with the Cr_3O-type, CsCl-type, $MgZn_2$-type, χ- or σ- phase structure. Although similarities in the alloying behavior of Tc and Re have been brought to light in the present study, the formation by Tc of Cr_3O-type and CsCl-type phases has no parallel in the alloy chemistry of Re.

A total of ten CsCl-type phases involving Sc has been discovered. The phases have the formula AB where A is Sc and B is an element from Groups VIII or IB. The lattice contractions, a measure of the bond strength, may be related to the total number of electrons of the B component outside the rare gas or 4f shell, suggesting that an electron concentration effect governs the occurrence and stability of these phases.

For the families of phases whose prototypes are CsCl, $MgCu_2$, $MgZn_2$, Cu_3Au, $TiNi_3$ and Cr_3O certain empirical relationships have emerged for predicting, in terms of the periodic table positions of the components, the compositions of the phases in binary systems, ternary systems and systems of higher order. Work is continuing to find similar relations for families of compounds whose prototypes are CuAu, CrB, FeB, AlB_2, Ni_2In, $TiCu_3$ and $TiAl_3$.

2. Thermodynamic Properties of Transition Metal Alloys

J. B. Darby, Jr. and K. M. Myles

It is the purpose of these investigations to attempt to correlate the thermodynamic properties of certain transition element binary alloys with the important atomistic factors of size, electronegativity, and valency. Furthermore, knowledge of these properties will be of considerable value in the interpretation of data accumulated on the same alloy systems by other experimental approaches such as magnetization measurements and nuclear magnetic resonance studies.

Enthalpy measurements will be conducted in a liquid-metal solution calorimeter which has now been assembled and which will soon become operational. The calorimeter is of the twin "micro" type which will employ a liquid metal solvent such as tin or aluminum at temperatures up to 750°C. Information on the kinetics of solution of the first long period elements in the liquid metal solvents has been obtained. When the calorimeter has been calibrated and is considered ready for experimental work a noble metal binary system will first be investigated to gain experimental confidence. Then transition metal systems will be studied.

The thermodynamic properties of the vanadium-iron system have been determined at 1600°K by the torsion-effusion method. Large negative deviations of the activity from ideal behavior have been found for both iron and vanadium. Although the experimental technique does not permit a highly precise determination of the temperature coefficients of the activity, it is reasonably certain that large positive excess entropies characterize the alloys. These observations suggest that a strong attractive force exists between the vanadium atom and the iron atom. Preparations are being made to extend the study to the vanadium-chromium system.

3. Electronic Structures of Solid Solutions and Intermediate Phases
A. T. Aldred and D. J. Lam

Magnetic susceptibility measurements provide a powerful tool for determining the electronic configurations of solid solution alloys and intermediate phases. The primary emphasis is currently placed on an exploration of the electronic density of states of alloys of the first and second long period transition elements. Recently, the magnetic susceptibilities have been measured over the whole composition range in the V-Tc and Nb-Tc systems. The results indicate that the rigid band approximation is valid for the b.c.c. solid solution region and that there is little or no localization of d electrons. Work is continuing in these and other transitional alloy systems.

A significant question which has arisen in the analysis of susceptibility and Knight shift data is the identification of the wave function character of the electrons at the Fermi surface. While certain deductions as to the relative concentrations of electrons in s and non-s states may be made from present information, measurements of spin-lattice relaxation time can provide an exact definition of the fraction of electrons having s-character. A nuclear magnetic resonance pulse apparatus suitable for the study of spin-lattice relaxation time and free induction decay shape is now under consturction. It is believed that this facility will provide clarifying information on wave function character, as well as serve as a source of additional independent physical measurements pertinent to our interests in electronic structure.

Another approach which is being followed to provide an insight into electronic structure is the measurement of thermoelectric power. Although this property is to some extent structure sensitive, it is a measure of the electronic density of states in an alloy. High temperatue (0-800°C) thermoelectric powers have been determined for Pd-rich solid solutions in the systems Pd-V, Pd-Cr, Pd-Mn, Pd-Fe, Pd-Co and Pd-Ni. Initial results indicate the possibility of a correlation with the theoretically proposed density of states curves. In the system Fe-V measurements have revealed a complex dependence of thermoelectric power on temperature and composition which cannot be analyzed until work on U-rich alloys is completed.

4. Nuclear Magnetic Resonance Studies in Metals and Alloys
D. J. Lam and D. O. Van Ostenburg

Nuclear magnetic resonance has been proven to be very useful in the study of the electronic structure of metals and alloys. The primary emphasis in which we are currently engaged is to explore environmental and electronic changes on alloying in substitutional solid solutions and intermetallic compounds.

Recently, the nuclear magnetic resonance of Tc^{99} has been observed in Tc metal and quadrupolar measurements indicate that the conduction electrons are distributed nearly spherically symmetric about each nucleus. Knight shifts of the Tc^{99} nucleus have been measured over the whole compostion range in the V-Tc system and correlated with magnetic susceptibilities. In addition, Knight shifts of the V^{51} isotope have been measured in binary alloys of V with Ti, Cr and Tc. The results on these b.c.c. alloys indicate that the rigid band approximation is valid and nearly all electrons outside the closed 3p or 4p shell form a common conduction band with admixtures of s and non-s electronic states. Furthermore, this data augmented by electronic specific heat measurements indicate that the proportions of electrons having s and non-s character changes with electron concentration within this common conduction band. Work is continuing in these and other transitional alloy systems to acquire a basic theoretical understanding of the electronic and structural properties of solids.

5. Ferromagnetism in Transition Metal Alloys
A. T. Aldred and M. V. Nevitt

Experimental observations of the occurrence and magnitude of atomic magnetic moments in transition metal alloys provide a powerful technique for understanding the electronic structures and bonding characteristics of these alloys. Measurements on Fe-V solid solutions indicate that on adding V to Fe the magnetic moment decreases at a rate faster than that corresponding to dilution of a constant Fe moment. This implies a decrease in the Fe moment and thus an apparent electron transfer effect between Fe and V. Transformation of alloys in the equiatomic composition range to the metastable CsCl structure produces a 20 percent decrease in the moment, while further transformation to the stable σ-phase diminishes the moment by about a factor of three. This decrease apparently reflects the change in atomic ordering. Preliminary measurements on other Fe-base alloys indicate that while alloying Fe with a nontransition element (Be,Ga) produces a dilution effect on the magnetic moment, the moment decreases more rapidly in alloys with the early transition elements (Mo,W). Further work is currently in progress.

6. Phase Relationships in Systems of Thoride Elements with Carbon
S. Rosen

Information on the electronic structure of the elements of the 5f series can be derived from a knowledge of their behavior with a nonmetal having rather well-established covalent and ionic bonding characteristics such as carbon. Furthermore, significant comparisons can be made between the electronic states in th 5f metals and in the 3d, 4d, and 5d transition metals by studying the conditions under which they form isostructural carbides.

The investigation of the U-Pu-C system up to 50 a/o carbon has been completed. Interest has been heightened by the observation of a transition from stoichiometry to nonstoichiometry, as regards the carbon content, in the NaCl-type phase (U,Pu)C, a situation also found in certain other isostructural monocarbide phases. It is believed that the transition may have its origin in an electron concentration effect, with carbon acting as an electron donor. An extension of the study is in progress which includes sections of the quaternary U-Pu-Th-C system containing around 50 a/o carbon and also includes a number of pseudo-binary systems of the monocarbides of transition metals which have the NaCl-type structure. It is probable that information regarding the valences and the distribution of electronic states in the thoride elements will be obtained from a systematic study of multicomponent systems of transition metals and thoride metals.

7. Miscibility of Laves Phases
J. B. Darby, Jr. and D. J. Lam

The immediate aim of this work is to investigate the solubility ranges of Laves-type phases in certain ternary systems in which two of the limiting binary systems contain the phases. When restricted mutual solubility is found an attempt is made to correlate the limiting solubility with factors such as relative atomic size, electronegativity, and valence electron concentration. The system displaying a complete range of solid solubility between the binary phases will be utilized in a quantitative study of the electronic relationship between uranium and the transition elements of interest. This will include various property measurements over the range of stability.

Ternary systems in which the phase relationships have been established include the $U(Fe,Al)_2$, $(U,Hf)Al_2$, $(U,Zr)Al_2$, and $U(Fe,Co)_2$. There is a complete range of solid solubility between UFe_2 and UCo_2.

8. Superconducting Transition Temperatures of Cr_3O-Type Ternary Phases
S. T. Zegler

This program is concerned with the superconducting properties of metals, solid solutions and intermediate phases. The objective is to elucidate the dependence of superconducting properties on crystallographic and electronic parameters as well as upon purity and homogeneity. Initial work is being directed toward determining the superconducting transition temperatures of Cr_3O-type ternary phases as a function of cyrstal lattice dimension, valence electron concentration and atomic mass and volume.

The construction of an apparatus for measuring transition temperatues in nearly zero field is now nearing completion.

Equilibrium studies are being conducted to find solid solution fields of the Cr_3O-type phases which can provide critical tests of atomic size and electronic effects. Crystallographic data have been obtained indicating that the Cr_3O-type phase V_3Co exhibits extensive solid solubility for Ni,Rh and Ir while Nb_3Rh exhibits limited solubility for Co, Ru, Pd and Ir. There is some solubility of Sb in Nb_3Sn; V_3Si and V_3Ga are soluble in all proportions.

C. Neutron and X-ray Diffraction Studies

S. S. Sidhu

The major emphasis of this work is on the determination of structure properties of materials both in the solid and the liquid states by combined neutron and x-ray diffraction techniques. It is aided by a number of computer programs which have been written or placed in operation, and which permit the best determination of a number of crystallographic variables such as atom position parameters, reciprocal lattice positions, lattice constants, interatomic distances, percent occupancy of crystal lattice sites by different atoms in a compound, nuclear coherent scattering amplitudes, etc., as well as Patterson and Fourier maps used in solution of crystal structures. The diffraction apparatus which have been completed in the past year are a Neutron Diffractometer (instrument which moves in a vertical plane and utilizes the same beam as used by the horizontal Spectrometer), the suitable Soller slit collimators and a drive for α-2α motion for the analyzing crystal used in studies of crystal dynamics, and a goniostat.

Investigations which have been recently completed and those that are currently in progress include the following:

1. Magnetic Structure Studies

a. Crystal Structure Variations in Alpha Uranium at Low Temperatures (M. H. Mueller). The unusual temperature dependence of the elastic modulii and other physical properties of alpha uranium near 43°K which have been previously reported are found to be correlated with changes in atomic positions and unit cell dimensions. The atom position parameter, y, decreases to a minimum at 43°K then rapidly rises on further cooling, as shown both by X-ray and neutron data. The a_o and b_o cell dimensions decrease to a minimum at 43°K and then rapidly increase in the range 43-18°K; the c_o dimension contracts on cooling to 43°K and decreases even more rapidly below this temperature.

Neutron diffraction studies of single crystals have now revealed the existence of additional reflections at room temperature and below which may be due to a magnetic change. Several reflections, including the (001) and (003), have been detected with intensities several times that attributable to the /2 component of the beam which are not observed in the X-ray pattern. Further work is in progress to find other observable additional reflections, their temperature dependence and their possible explanation on the basis of a magnetic arrangement.

b. Atomic and Magnetic Ordering in MnCo and $(Mn,Co)_4C$. N. S. S. Murthy and S. S. Sidhu). MnCo alloy annealed at 1223°K for 300 hours and cooled to room temperature at a rate of 1°C per minute showed considerable ordering (50 percent) at this temperature, the face-centered cubic unit cell of a_o = 3.615Å, having Mn atoms at 0 0 0, 1/2 1/2 0 and Co atoms at 1/2 0 1/2 and 0 1/2 1/2. It disordered at approximately 800°K. The magnetic ordering appeared at 263°K, with magnetic moments of Mn atoms aligned oppositely to those of Co atoms. An unannealed sample of the same alloy showed no appreciable ordering of either variety even down to 20°K. It thus shows that both the atomic ordering and the Neel temperature are influenced by the annealing temperature.

In the cubic unit cell of $(Mn,Co)_4C$, (a_o = 3.78Å) the carbon atom occupies 1/2 1/2 1/2 site. The metal atoms occupy 0 0 0, 1/2 1/2 0, 1/2 0 1/2 and 0 1/2 1/2 sites with MnI at 0 0 0, and 2 Co and MnII distributed randomly at the remaining sites. The carbide is ferrimagnetic at room temperature with the magnetic moments aligned as Mn(I)↑ , 2 Co↑ and Mn(II)↓.

2. Crystal Structure Studies

a. Zirconium-Deuterium System (N. S. S. Murthy and S. S Sidhu). A systematic study of zirconium-deuterium system in the composition range of 2 to 66.5 atomic percent deuterium shows that the system at room temperature con- in addition to α-Zr three nonstoichiometric phases, (γ, δ, ϵ). The crystal structures of the δ and the ϵ phases have been determined by several investigators and are available in literature. The identity, crystal structure, composition range of existence and the transformation temperature of the γ-phase were not well known, nor were the mechanisms of transformation of α-Zr into the γ-phase, and the γ-phase into the δ-phase. Diffraction studies and metallographic examinations showed that the γ-phase was formed in the composition range 0-10 atomic percent deuterium and coexisted with α-Zr at room temperature. There was no evidence of the formation of the δ-phase in this range. Alpha Zr, γ and δ phases are present in the composition range 10-50 atomic percent D, and the γ and δ phases in 50-60 atomic percent D. The γ-phase is tetragonal with a_o = 4.586Å; c_o = 4.948Å and C = 1.08. There are four (ZrD) molecules per unit cell having

4 Zr at: 0 0 0; 1/2 1/2 0; 1/2 0 1/2; 0 1/2 1/2

2 D at: 1/4 1/4 1/4; 3/4 3/4 3/4

2 D at: 1/4 1/4 3/4; 3/4 3/4 1/4.

The mechanisms of transformation of α-Zr into the γ-phase, and the γ-phase into the δ-phase have been determined. In view of the results obtained in this investigation an evaluation of the existing concepts of interstitial solid solutions of deuterium (or hydrogen) in α-Zr is given.

b. Coordination Compound (M. H. Mueller and S. H. Simonsen). The crystal structure of disodium tetranitritonitrosohydroxyruthenate (III) 2-hydrate is being investigated using three-dimensional neutron diffraction data (about 2000 reflections) and zone X-ray data. The crystal is monoclinic with a_o = 12.75, b_o = 14.52, c_o = 7.37Å, β = 121.2°, Dm = 2.29g cm^{-3}, assuming four molecules per unit cell. Systematic extinctions were found for h+k = 2n+1, so that the possible space groups are C^2, Cm, or C^2/m. The N(z) test was applied to the neutron data and the results clearly indicated the most probable space group to be C^2/m.

The positions of the Ru, O of the hydroxyl, and N's and O's of the NO and NO_2 groups were recovered from the three-dimensional Patterson synthesis, using Buerger minimum functions. The Na's and also the O's of the waters were found by Fourier methods using X-ray zone data, with signs based on parameters derived

from the neutron Patterson synthesis. Two to three cycles of l.s. refinement yielded agreement factors, $R = \Sigma (|F_o| - |F_c|)/ \Sigma|F_o|$, of .28, .16, and .26 for the (h0ℓ), (0kℓ) and (hk0) zones, respectively. The hydrogens will be located by three-dimensional Fourier methods, based upon the above model, and the structure will be refined by least squares.

c. Oxides (M. H. Mueller). The crystal structure studies of Ti_2Ni, Ti_4Ni_2O, and Ti_4Cu_2O have been completed. These structures are cubic with an a_o of approximately 11.3Å and 96 to 112 atoms per unit cell dependent upon the percent oxygen. A neutron diffraction study has confirmed the X-ray results on the relative positions of the Ti and Ni atoms in Ti_2Ni and has shown that the oxygen enters into unoccupied sites existing in the basic Ti_2Ni structure.

3. Liquid Metal Studies
LeRoy Heaton and Clifford Thompson

Liquid solutions of cesium and sodium metals over the range of compositions from pure cesium to pure sodium were studied with neutrons in the temperature range of -20°C to 365°C. The patterns are being interpreted to determine the distributions of the like and the unlike nearest neighbor atoms in the solutions.

4. Thermal Neutron Coherent Scattering Amplitudes
M. H. Mueller

Coherent nuclear scattering amplitudes for some of the nuclei have been determined and are as follows:

Isotopic Composition	$b_{coh.}$ (10^{-12}cm)
Os^{188}	0.78
Os^{189}	0.90
Os^{190}	1.09
Os^{192}	1.34
Tc (element)	0.60 (preliminary)
Ir (element)	1.05 (redetermined)

The redetermined value of the amplitude for iridium was based on IrO_2. The previous value, b, for Ir was 0.36 x 10^{-12}cm. A continued effort in this area is planned as elements and isotopes become available.

D. Irradiation Effects in Metals

1. Low Temperature Irradiation Effects
T. H. Blewitt

The high mobility of radiation induced defects requires the utilization of very low bombarded temperatures for the fundamental study of irradiation damage. The first phase of this work is therefore the design and completion of low temperature irradiation facilities. These are being built in the CP-5 reactor and will

allow bombardments to temperatures as low as 3.5°K in a thermal neutron environment of 10^{13} neutrons per cm^2 per second and less than 10^{10} neutrons per cm^2 per second of epithermal or higher, or in a neutron environment of 3×10^{11} fission neutrons with less than 10^9 thermal neutrons. The scope of the research involves a variety of in situ measurements including stored energy, electrical resistivity, length change measurements in nonfissile metals such as the noble metals, especially with regard to dose dependence effects in the high dose regions. The fissile materials will also be studied, particularly in regard to irradiation growth.

2. Radiation Effects in Anisotropic Solids
B. Loomis

The purpose of this research is the study of the effect of irradiation on anisotropic solids. The initial portion of the work has been the study of the effects of fission fragments (0.1 to 0.3 a/o burnup) on the swelling of β-quenched uranium alloys. This work is being extended to included alpha recyrstallized uranium and single crystals of uranium. The properties to be measured are density and electrical resistivity. Observations of the microstructure utilizing electron microscopy techniques will also be made. Irradiation induced growth will be studied utilizing the low temperature facility now being completed in the CP-5 reactor. In these experiments growth will be investigated in fissile materials, such as uranium and uranium-doped zirconium and in nonfissile anisotropic materials, such as zinc, bismuth and magnesium. In the latter case energetic neutrons will be used as the bombarding particle. Properties to be measured will be length changes in various crystallographic directions and density.

3. Transmission Electron Microscopy Studies of Fission Fragment Damage in Solids
R. K. Hart and K. Merkle

The purpose of these studies is to determine the mechanism of defect formation and the nature and number of defects created by fission fragments passing through the solids. Current experiments have been primarily concerned with the criteria of fission track formation in a variety of solids including the noble metals, platinum, and some oxides. Current results indicate that particle size of the thin film plays an important role in the appearance of fission tracks. In some instances, usually in transmission experiments with large crystallities, isolated black spots indicative of local stress appear instead of fission tracks. Subsequent experiments will extend current work dealing with the nature of these spots. Of particular interest will be annealing experiments for the electrical resistivity measured in conjunction with the transmission electron microscope studies. It is also anticipated that low temperature studies will also be initiated.

4. Irradiation and Solid Solution Strengthening Effects of Copper Single Crystals
T. Koppenaal

The purpose of these studies is the investigation of strengthening mechanisms in copper single crystals using a high sensitivity strain detector to determine flow stresses. The strain detector to be used in these experiments is capable of measuring the strains of 10^{-6} inch per inch. The strengthening mechanisms to be studied will be irradiation effects and alloying. In these experiments the yield stress as determined from the nonlinearity of the stress-strain curve will be measured. Of particular interest will be the study of strengthening in an alloy by irradiation.

The irradiation experiments will be conducted at bombardment temperatures ranging down to 4.2°K, and annealing studies ranging from this temperature up to 700°K will be made. At higher temperatures etch pit investigations will be used to determine dislocation densities and the temperature dependence of the stress required to activate the dislocation.

5. Effect of Neutron Irradiation on Precipitation

J. Horak

The purpose of this research is to investigate the effect of irradiation induced defects on the precipitation process. Although it is intended to study all of the phases of precipitation, the initial experiments will be conducted on the study of the decomposition of supersaturated solutions. The samples will be bombarded at temperatures below that where normal bulk diffusion can occur, and the influence of the irradiation generated vacancies and interstitials will be studied. Aluminum based copper alloys will be the first materials to be studied. The decomposition will be monitored by electrical resistivity so that kinetics of the decomposition as a function of point defect concentration can be studied. Small angle scattering and electron microscopy will also be used to obtain information in regard to the structural changes occurring. Subsequent studies will involve alloys which precipitate a magnetic phase in order to utilize magnetic measurements in the study of the heterogeneities in the solid solution.

E. Corrosion Research

J. E. Draley

The overall objective of the present program is to understand the mechanism of the corrosion of metals in water. From time to time the work extends into other environments such as oxygen and steam, and into the effects of other constituents dissolved in water. It is believed that in all or nearly all of these cases resistance to corrosion is provided by oxide films which are quite thin, and which are remarkably tightly bonded to the metal substrate and remarkably resistant to the to the passage of reactants or reaction products.

The films are not stable in the corrosive environment and suffer various forms of degradation, which influence and can be said to determine the corrosion resistance imparted by the films. Some of the forms of this degradation are transformation to more stable crystal structures, breakdown into well ordered crystallites, hydration (or hydroxylation) into more stable (in the environment) modifications, and cracking or breaking.

A special case of film degradation or damage is that due to hydrogen. Protons doubtless enter the films from hydroxide adsorbed on the outer surface and are transported through as part of the corrosion reaction. The permeability and stability of the film are thus influenced, the nature of the substrate surface is often affected by the hydrogen formed there, and the hydrogen sometimes ruptures the film in order to escape.

1. Electron Optical Study of Surface Reaction Products
R. K. Hart

One important aspect of metallic corrosion and oxidation is a thorough understanding of physical attributes of the metal and structural relationship between these and the overlying reaction product. Thus a detailed knowledge of the physical relationship between metal and compound (s) by itself and more importantly tied in with other investigations such as kinetic studies and electrochemical or chemical behavior, will lead to a better understanding of the problem.

Elucidation of any corrosion problem is complex because nearly all systems are "dirty" systems and thus many variable have to be taken into account.

In this program, electron optics is playing its part in clearing up some of the controversial aspects of the subject, based on observations in the corrosion of aluminum, iron and steels, and zirconium. The epitaxial and nonepitaxial relationships rather than due to misfit between the two lattices as originally postulated. From the number and type of crystallographic features one sees in oxide films it appears that surface diffusion to favorable sites plays a more important role than hitherto realized. Another interesting feature that electron optics has brought to light is that oxide overgrowth is not necessarily dependent on defect structures at the metal surface and that surface finishing treatments and impurities are often more important.

2. Oxidation of Zirconium
R. D. Misch

The objective is to determine the mechanism by which a solid reaction product develops between a metal and a gas. Many features of this mechanism are not understood, in particular for metals such as zirconium. These include the cubic law of oxidation, transitions from one rate law to another and the dependence of this behavior on the presence of water vapor. By closely relating the EMF which develops across the growing oxide scale on zirconium and its structural features the growth mechanism can be identified.

Measurements of the EMF of the scale formed on zirconium in oxygen have indicated that the oxidation is equally controlled by ionic and electronic conduction in the scale. Oxidation rates for a series of alloys in oxygen and steam are related if one takes into account the emf of the scale. The accelerating effect of steam on the oxidation rate of zirconium and zirconium alloys is a minimum if the EMF is low (e.g. Zr - 2% Fe) and a maximum if the EMF is high (unalloyed Zr). Oxidation in steam introduces the possibility of protonic conduction in the oxide and hydrogen absorption by the metal. The EMF results show that the oxidation accelerating character of hydrogen is minimized by an increase in electronic conductivity.

The interpretation of electrical measurements requires a knowledge of the homogeneity of the scale which frequently contains cracks and second phases. The present program is designed to separate some of these factors in the case of zirconium by comparison of the X-ray, metallographic and EMF characteristics of the oxide scale at critical stages in its development.

3. The Kinetics of Aqueous Aluminum Corrosion
S. Mori

The chemical and physical aspects of corrosion are being studied as a means determining the mechanisms of the corrosion of aluminum in water. The presence of oxide films and the local nature of the reaction indicate that rate control is related to local degradation and repair of corrosion product oxide. Determination of the amount of metal corroded, the weight of the adherent corrosion product, and the amount of product lost to the water permits calculation of the composition of the corrosion product coating.

Careful measurements have shown that during two periods the amount of corrosion of "commercially pure" aluminum varies with the logarithm of time. Between these two periods, there is a break upward in the corrosion curve. The logarithmic behavior has been interpreted in terms of alternate film growth and breakdown, with the latter perhaps induced by the accumulation of corrosion product hydrogen beneath the protective film.

The break in the curve depends on surface preparation and contamination of the water close to the corroding surface. Measurement at a distance of 0.1 mm from the surface has shown pH values as high as 10.2 and as low as 1.5 in water which is quite pure in the bulk. The reactions responsible for this are being sought.

4. The Aqueous Corrosion of Aluminum Alloys at Elevated Temperatures
W. E. Ruther

The use of rapidly flowing water as a corrodent is proving to be a valuable tool in elucidating the mechanism of aluminum corrosion at elevated temperatures. Environmental effects, which are either absent or lost in the experimental errors in static water, become very important in dynamic corrosion. Explaining these effects should provide a better general understanding of the interactions at the water-aluminum oxide interface during corrosion.

Corrosion tests have been completed in which different aluminum alloy systems, oxygen levels, analyses of flowing stream solids, surface areas, flowing path length and changes in stream temperatures have been variables. From the results of these tests it has been tentatively postulated that precipitation and adherence of a colloid (usually but not always a form of aluminum oxide) on the outer surface of the protective oxide film is essential to a low aluminum corrosion rate.

The source of the colloid is assumed to be the neutralization of alkaline (or acid) streams (carrying the aluminum in a soluble form) issuing from cracks and fissures in the protective oxide. This mechanism seems to have validity for the corrosion of aluminum under other conditions as well.

In current tests, colloidal species are injected just upstream of the aluminum specimens and the effects on the corrosion rate are measured. The deposition of corrosion products as a function of position in the loop are also being studied.

5. Polarization Studies
J. E. Draley

Since the processes occurring during aqueous corrosion involve the transfer of charge, the interrelationships between overall current flowing, the potential, and the corrosion rate allow the deduction of the important steps in the corrosion reaction. Variation of the basic parameters while making the measurements should make it possible to deduce the roles of the various processes in controlling corrosion.

Methods of measurement have been developed and polarization curves have been determined for almost 20 pure metals in boiling distilled water. Work has begun on determining fundamental curve shapes for reactions on aluminum, and the deduction of corrosion mechanisms from polarization curves.

F. Physical Ceramics Research

1. Dislocations and Neutron-Induced Defects in Oxides
P. F. Stablein

The purpose of this research is the study of the interaction of point defects and dislocations in oxides. The initial work in this research is concentrated on the study of neutron irradiated magnesium oxide single crystals. The investigation of the interaction of dislocations with irradiation induced defects was studied using dislocation etching techniques on samples deformed by bending and by hardness identations. Analyses of these in conjunction with slip line traces were made to determine dislocation generating stresses and dislocation movement stresses. Annealing phenomena have also been studied. This work will be extended to include additional annealing experiments so that the annealing kinetics can be determined. Studies of dose dependence and the dependence of the energy of the bombarded particle on the mechanical properties of MgO will also be undertaken. It is anticipated that cobalt, nickel and iron oxides will be investigated in the subsequent phases of this research. Of particular interest in the case of iron oxides will be the study of nonstoichiometry on dislocation generation and mobilities.

2. Determination of Work Functions
C. A. Arenberg

The purpose of this work is the accurate investigation of the work functions of both metal and ceramic material surfaces. These will be measured by the utilization of a field emission microscope. This technique enables the determination to be made to a high degree of accuracy, as clean regular surfaces can readily be prepared in the microscope. The variation of the work function with the crystal face will also be measured. Initial work is concerned with platinum and gold to establish reliability of method, to be followed by studies on ceramic material surfaces.

3. The Effect of Surface Defects and Topology Upon the Catalytic Activity of Solid Oxides

M. L. Volpe

The purpose of this research is to determine quantitatively the relative importance of structural factors of ceramic materials in catalysis. Most investigations on catalysis by solids have stressed the importance of the electrical properties of the catalyst. Of those that have been concerned with the effect of crystal structure on catalysis there have been only a few om which the catalyst surface has been well defined and they involved metallic rather than ceramic catalysts.

Since experiments on powders have indicated that in the MgO catalyzed decomposition of N_2O structural factors are more important than electronic ones, and theory has supported this contention, this reaction was chosen for the present work. Thin, single crystal wafers of MgO having well-defined surfaces will be used; the reaction rate will be measured as a function of crystallographic orientation, surface density of both point and line defects, and surface roughness. Surfaces will be prepared by both cleavage and by mechanical polishing followed by chemical polishing. The crystals will be annealed at elevated temperatures in an ultra high vacuum. After annealing, controlled amounts of point defects will be introduced by irradiation; dislocations will be produced by mechanically stressing the crystals. The dislocation density will be measured by selective etching; the point defect concentration will be estimated by hardness impressions. Electron-microscopic examination of the surfaces, both before and after reaction, will be made.

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Contractor: Argonne National Laboratory, Argonne, Illinois

Contract Number: W-31-109-eng-38

Present Contract Term: July 1, 1962 through June 30, 1963 (Fiscal year 1963)

Cost to AEC: $2,046,000

Contract Title: PHYSICAL RESEARCH IN THE SOLID STATE SCIENCES DIVISION

Investigators: O. C. Simpson, Director, Solid State Sciences Division and staff

Scope of Work: A. Application of Resonance Effects to the Study of Solids

1. Optical and Spin Resonance Properties of Single Crystals - Color Center Research
C. J. Delbecq, G. Kuwabara, F. Phelps, S. Susman and P. H. Yuster

Studies are being made of the optical, electron spin resonance, electrical, thermal and photoconductive properties of doped and undoped alkali halide crystals after low temperature irradiation with ionizing radiation. The purpose is to elucidate the role played by the hole and hole traps as well as by the electron and electron traps in determining the characteristics of the defect centers and their inter-relations. Certain specific projects now underway are as follows:

The nature of the centers formed after X-irradiation as a result of hole trapping is being studied in mixed crystal systems such as KCl-KBr and KCl-KF. It has already been shown, through the use of ESR that species such as $BrCl^-$ and FCl^- are formed. It has also been shown in the KCl-KBr (1000:1) system that $BrCl^-$ is more stable thermally than Cl_2^- and that Br^- is a better trap for a positive hole in KCl than is Cl^-. There are indications that the fluorine nucleus is interstitial in FCl^- and therefore such studies may supply information regarding the production of Frenkel defects in these crystals.

Pure KCN has been prepared and the color centers produced in this material, which has the alkali halide structure, are being studied. Color centers analogous to the F- and M- centers in the alkali halides are observed.

The kinetics of formation of M-centers in KCl (presently believed to be two associated F-centers), are being studied. Correlated with this work is a study of the yield of F-center luminescence as a function of M-center concentration. It is hoped that these studies will yield information regarding energy transfer in these crystals.

2. Electron and Nuclear Magnetic Resonance Studies

E. Avery, D. Connor, D. Davis, J. Gabriel, D. O'Reilly, G. Schacher, B. Smaller and T. Tsang

Electron and nuclear resonance techniques have proven to be invaluable aids in investigations of many basic problems particularly in the study of radiation effects and in the study of crystalline field effects.

a. Electron Spin Resonance (E. Avery, J. Gabriel and B. Smaller). The electron paramagnetic resonance technique is being used to investigate the triplet state properties of organic phosphors. The electron-electron dipole interaction and electron-nuclear interaction has been investigated for several of these S=1 species. Studies of the energy transfer mechanism between the triplet states is given emphasis. These studies have especial significance in such diverse fields as organic LASERS, photochemistry involving excited states, radiation sensitizing processes and biological energy transfer problems. The e.p.r. technique enables one to determine independently and unambiguously the triplet state concentration of each component in a complex system.

b. Nuclear Magnetic Resonance of Stable or Long-Lived Nuclides (D. O'Reilly, T. Tsang and G. Schacher). Work is continuing on the Knight shifts of Li^7 and Na^{23} for solutions of Li and Na in liquid ammonia. These results will be correlated with measurements by spin-echo techniques of electronic spin-lattice relaxation times. Structures of solids are being determined by measurements of the anisotropy of the NMR line shapes coupled with analysis by the moment method. Previous work on the rate of exchange of I^{127} with $HgI_4^=$ and $HgI_3(OH_2^-)$ is being slightly extended by an investigation of allied systems. Temperature and concentration dependences of these reactions are under investigation. Rates and activation energies will aid in further knowledge of the mechanism of the exchange reactions. Electron-nuclear double resonance studies of the coupling of unpaired electrons with nuclei of host crystals containing paramagnetic impurities are being undertaken in order to determine the magnitude of unpaired electron wave functions at nuclei of the host crystal as well as (longer range) dipolar couplings between electrons and nuclei.

c. Nuclear Magnetic Resonance of Short-Lived Nuclides (D. Connor and D. Davis). Study of the nuclear magnetic resonance of a number of nuclides too short-lived for investigation by conventional methods has been made possible by a novel technique developed at Argonne. Anisotropy in the beta-decay of polarized nuclei serves to measure the large nuclear polarization (order ten per cent) of sample nuclei resulting from the capture of polarized neutrons. Changes in the nuclear polarization due to the interaction of the nuclear magnetic moments with an applied radiofrequency magnetic field are observed via the anisotropy, so that resonance experiments are possible. The magnetic moments of Li^8 and F^{20} have been measured in this manner, sign as well as magnitude being obtained through the use of polarized r.f. fields. The study of many more nuclides will be possible with a recently completed cryostat which permits holding the sample temperature at 80°K with a resulting great increase in relaxation time of the nuclear polarization. The nuclei observed in experiments of this sort have

each taken part in a radiation-damage event due to the nuclear recoil associated with emission of the neutron-capture gamma ray. Since the resultant lattice damage affects the shape of the resonance line, studies of the latter should provide some information about radiation-damage mechanisms. A preliminary study of the angular dependence of the line width for F^{20} in CaF_2 indicates that few if any recoiling nuclei come to rest in interstitial positions. Further work of this sort, particularly at low temperatures, may shed some light on the microscopic aspects of radiation damage, now almost unknown experimentally.

3. Solid State Mössbauer Experiments
J. Mullen

A study of vacancy-impurity association is being made through observation of the quadrupole splitting of Fe^{57m} in NaCl. Theoretically, the parent of Fe^{57m}, i.e., Co^{57}, should have a positive ion vacancy associated with it in order to maintain charge neutrality. Observed splittings of the spin 3/2 state of Fe^{57m} would constitute direct evidence for the expected association. Preliminary measurements appear consistent with the theory. Measurements as a function of temperature should yield vacancy-impurity binding energies.

In another experiment an attempt is being made to observe the anisotropy in the fraction of recoilless radiations from Sn^{119}, as predicted by the Debye-Waller theory.

B. Experimental Studies of Material Classes

1. The Physical and Chemical Properties of Graphite
W. Bollmann, M. Dzurus, G. R. Hennig, M. Kanter and G. Montet

The objective of this work is to increase the basic understanding of the solid state physics and chemistry of crystalline carbon, especially of graphite. A large part of the research deals with single crystals of natural origin since these are the best crystalline materials available to date. However, radiation damage studies are also being carried out on polycrystalline pile grade graphite.

Considerable emphasis is given to the use of electron microscopy to study defect structures. Diffraction studies on thin lamellae have made it possible to identify various defect structures whose presence had been postulated to explain physical and chemical properties of graphite. The structures found in irradiated graphite are being correlated with those introduced by quenching or by mechanical deformation.

The physical and chemical properties of graphite are considerably altered when small amounts of boron are dissolved in the lattice. Under certain conditions, dislocation loops appear and possibly also minute precipitates. These effects are under further study by electron microscopy.

Electron microscopy is also being used to study radiation induced decomposition and polymerization reactions. Such reactions could be used for high resolution autoradiography and might be applicable to tracer diffusion studies in graphite.

Mössbauer measurements are being used to determine the mobility and bonding of impurities in graphite. Lamellar and residue compounds of graphite containing iron or cobalt are being studied.

Many physical measurements require graphite crystals of larger size and perfection than those now available from natural sources. Therefore, the growth of crystals from solution in iron and in aluminum is under investigation.

2. Low-Temperature Radiation Effects in Hydrogen Bonded Glasses
J. A. McMillan

The purpose of this research is to investigate the correlation between the annealing of radiation damage and the thermal behavior during warm-up of hydrogen bonded glasses. The results will contribute to the understanding of the annealing kinetics and may have some practical importance in connection with radiation effects in solid rocket propellants.

Current work includes studies of the conditions of glass formation by supercooling, vacuum deposition of a vapour, and collection from a molecular beam; the thermal behavior during warm-up; and the radiation effects and their annealing as related with the thermal properties.

Substances covered by the present investigation are oxygen and nitrogen hydrides (water, hydrogen peroxide, hydrazine and derivatives), alcohols, amines and miscellaneous compounds, both in the pure state and in binary mixtures. The techniques used include Electron Paramagnetic Resonance and Thermal Analysis. Infrared studies will also be appleid to determine the stretching frequencies of the hydrogen bond in the vitreous states of aggregation of the substances under study.

3. Physics of Metals
G. Arai, S. Eckstein, Y. Eckstein, L. Guttman, J. Jackson, J. Ketterson, E. Yasaitis

The general objectives of this program is to gain a more thorough understanding of metals and alloys especially with respect to their electronic structure, defect structure and radiation damage, their order-disorder and phase transformation properties, and their atomic diffusion processes.

a. X-Ray Diffraction Studies (G. Arai and L. Guttman). The experimental program emphasizes the use of x-ray diffraction techniques for the study of atomic distributions in alloys or other solid solutions near phase transitions. The Al-Zn system is under study and will be followed by studies of other systems such as NaCl-KCl, the Fe-Al system, and possibly some partially miscible binary liquid system.

b. Fermi Surface Studies in Semi-Metals (S. Eckstein, Y. Eckstein, J. Ketterson, and E. Yasaitis). The Fermi surface of antimony and bismuth is under investigation by the methods of geometric resonance and de Haas-Shubnikov effect. The de Haas-Shubnikov effect is being studied in the ultrasonic attenuation and the

d.c. magneto resistance. Current measurements to 14,000 oe will soon be extended to 30,000 oe. Measurement of the "tilt effect" will allow a simultaneous determination of the Fermi velocity as a function of angle. Simple theoretical considerations show that when the drift velocity of electronic carriers exceeds the velocity of sound, amplification of sound should result. This amplification of sound has been calculated for semi-metals in crossed electric and magnetic fields. Experimental verification of the amplification is planned in semi-metals such as bismuth and in semiconductors. In addition, it is expected that we will be able to measure the Fermi velocity by using the tilt effect in amplification.

c. Point Defect Reactions in Platinum (J. Jackson). The effect on vacancy concentration of dislocation motion during quenches and at constant temperatures above 300°K has been determined in platinum. This work will be continued at lower temperatures. An attempt is being made to find vacancy pair binding energies by relaxation methods. The kinetics of aggregation of vacancies into larger clusters is being inferred from hardness measurements and will be observed by transmission electron microscopy. Study of the effect of massive plastic deformations on vacancy controlled diffusion is underway.

C. Interaction of Radiation with Matter

1. Inelastic Scattering of Subthermal Neutrons

D. Connor and J. Rush

The spectroscopy of cold (long wavelength) neutrons which have been inelastically scattered from a substance of interest constitutes a very powerful technique for the study of the dynamical properties of solids and liquids. The nature of the scattered spectrum depends on the details of the nuclear motions which, therefore, may be deduced from the observed spectra. For example, dispersion curves (relations between phonon wave vector and energy) and vibration spectra in crystals may be determined. Other phenomena which may be investigated via neutron inelastic scattering studies include spin waves in ferromagnets, diffusive motions in liquids and energy levels of paramagnetic atoms in crystals. Such studies will complement the theoretical studies already underway.

The experimental program just getting underway uses the conventional technique of beryllium-filter monochromatization, combined with chopper/time-of-flight spectrometry of scattered neutrons at 90°. Current development work should lead to later major improvements in resolution (mechanical velocity selector), neutron economy (simultaneous detection at several angles), and intensity (cryogenic moderator).

Two problems at present appear to be particularly suitable for early study. First, an experimental survey of scattering spectra from polycrystalline metals may lead to qualitative conclusions which will guide the development of lattice-dynamical theory as well as suggest important experiments of a more detailed nature. Second, we now know little of the dynamics of the amorphous solid state, making scattering studies of glasses very appealing. Measurements in the glass-liquid transition temperature range may also contribute to the elucidation of the thorny problems of liquid dynamics.

2. Radiation Damage to Various Solid Materials

W. Primak

The general goal of the program is a more thorough understanding of the mechanism of physical changes caused by corpuscular and energetic electromagnetic radiations in various solid materials. Physical properties such as electrical and optical properties have been studied. Special attention has been paid to dimensional changes which have been measured by a number of methods including precision density determinations, interferometry, and strain birefringence. Thermal annealing is also used as a tool of investigation.

Recent work has included the effect of temperature of irradiation on the electrical conductivity changes of artificial graphite (special emphasis on the damage dosimetry problem), the effect of temperature of irradiation in a gamma ray source on the expansion of lithium fluoride (separation of the F-center expansion from the 450-center expansion), proton and helium bombardment of silicon (demonstration of gas trapping in the crystal), separation of ionization and corpuscular radiation effects in the radiation induced dilatation of vitreous silica.

During the coming year greater emphasis will be placed on radiation effects associated with accelerated particles. The current program includes work with a cyclotron, positive and electron Van de Graaffs, and a Cockcroft Walton machine; and this will be extended to the use of a low energy ion accelerator currently under construction. Substances currently being studied are vitreous silica, quartz, and silicon. Other substances will be studied as techniques for their investigation are developed.

Annealing studies of the various effects discovered in vitreous silica are planned to provide a further characterization of the effects.

D. Low Temperature Physics

O. V. Lounasmaa and J. Mullen

The low temperature physics program includes the studies of the properties of liquid helium itself and precision low temperature calorimetric studies designed to obtain nuclear, lattice and electron contributions to specific heats. The low temperature physics group also operates the Collins liquifier and furnishes liquid helium to other groups.

Precision measurements of the thermodynamic behavior of helium-4 very near the lambda-curve are underway using temperature intervals of the order of 10^{-6} Preliminary results are already available.

A helium-3 cryostat is being used for low temperature specific heat measurements. During the past year measurements have been completed on six rare earth metals and on a few ferromagnetic alloys. Studies will continue as suitable samples become available.

A low temperature cryostat and velocity scanner for Mössbauer studies of internal fields is under construction. Results of these studies will be correlated with the results of the low temperature specific heat measurements.

E. Solid State Theory

T. Arai, P. Bagus, F. Bassani, D. Brust, F. Fumi, T. Gilbert, A. Rahman, J. Robinson, K. Singwi and M. Tosi

The solid state theory program has as its general objective the development of and application of new theoretical techniques and concepts and the application of existing methods and concepts to give a better understanding to the nature of solids. The program is intended to give a theoretical interpretation of experimental results and also to aid in the choice of the most important and fruitful experimental endeavors. All of the work reflects the specific interests and competencies of the staff members; some, however, are rather specifically tied-in with experimental research projects underway in the Division. The following projects are typical of the work:

a. Theory of Exchange Interaction in Magnetism (T. Arai). Exchange coupling of non-singlet atoms is being studied in order to obtain a rigorous justification of this concept, and to review the virtues and limitations of the Heitler-London method. The method is being generalized in such a way that atomic orbitals in crystals satisfy self-consistent requirements. A field theoretical description is being adapted to the method to facilitate calculation of correlation of d-electrons and interaction of d- and conduction electrons.

b. Electronic Structure of Semiconductors (F. Bassani and D. Brust). General O.P.W. calculations of the electronic band structures have been carried out for group IV and the III-V semiconductors at symmetry points of the Brillouin zone. The dependence of the results on the approximations to the crystal potential is being investigated. Using a semi-empirical pseudo-potential approach and the Bassani perturbation method, energy bands throughout the Brillouin zone have been computed in Ge and Si and compared with experimental data on interband transitions. The effect of alloying Ge with Si and applying hydrostatic pressure is being investigated.

c. Many-Body Theory in Crystals (F. Bassani and J. Robinson). The O.P.W. method has been generalized and incorporated in a one-particle Green's function formalism competent to treat many-electron effects in real periodic crystals. The formalism is being extended to include the electron-phonon interaction and attempts are in progress to apply it to numerical calculation of the cohesive energy of diamond and of the many-body effects on the energies and lifetimes of quasi-particle states in silicon and germanium.

d. Cohesion and Thermodynamic Properties of Ionic Crystals (F. Fumi and M. Tosi). Theoretical studies are underway in order to give a better understanding of the interionic forces and of the vibrational and defect properties of the alkali halide crystals. The theoretical equations of state, using various alternative forms of the force law, are being examined, and tested against the variation

of the cohesive energy with pressure, obtained from compression data at high pressures for alkali halides which do not undergo polymorphic transitions, against the experimental cohesive energy at atmospheric pressure, and against the experimental radii of ions in crystals, obtained from the measured maps of the electron distribution in crystals. An analysis of the pressure-volume relationship of alkali halide crystals for which polymophic transitions have been observed to occur has already provided direct evidence on the many-body character of the interionic forces. A review article on the Born theory of the cohesive properties of ionic solids is being prepared. The entropy, enthalpy, and heat capacity of alkali halide crystals, as functions of temperature, are being analyzed to study the range of validity of the quasi-harmonic approximation and the importance of strictly anharmonic effects in these solids, and to determine moments of their phonon frequency spectrum.

e. Ab Initio Calculations of Electronic Systems (P. Bagus and T. Gilbert). Accurate Hartree-Fock orbitals and energies for Ce have been calculated. Excited states and transition probabilities for selected light atoms will be computed and used to obtain a better estimate of the temperature of the sun's corona. Formal methods for bringing Hartree-Fock computations on solids (using the nonlocal exchange operator and iterating to self-consistency) within the scope of existing computing machines have been developed and will be coded shortly for machine computations. Calculations of the self-trapping energy and potential energy curves of the Σ_u and Σ_g states of a self-trapped hole (X_2^- or V_K center) are nearly complete. Calculations of the discrete excited levels which occur in x-ray emission spectra will be undertaken shortly. Calculations of the hyperfine structure of halogen molecule ions in crystalline fields (X_2^- and XY^- centers) are in progress.

f. Slow Neutron Scattering and Atomic Motions in Liquids (A. Rahman and K. Singwi). A stochastic model for diffusive motions in an assembly of interacting atoms has been postulated and used successfully to account for slow neutron scattering from water. This understanding is now being supplemented by simulating atomic motions on a digital computer using classical equations of motion, a simple interatomic potential and a convenient but not too small number of particles. The results up to date show that in liquid argon the diffusive motion is very similar to the motion of a Brownian particle. These calculations are now being refined and a larger variety of liquids is under investigation.

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Contractor:	Brookhaven National Laboratory, Upton, Long Island, New York
Contract Number:	AT(30-2) - Gen - 16
Present Contract Term:	July 1, 1962 through June 30, 1963 (Fiscal year 1963)
Cost to AEC:	$700,000
Contract Title:	BASIC RESEARCH IN THE METALLURGY DIVISION
Investigators:	D. Gurinsky and staff

Scope of Work:

A. Liquid Metals

1. Liquid Alloy Reactions
J. R. Weeks

Factors relating the structure, constitution, and thermodynamics of liquid alloys are being investigated. Experiments underway or proposed include precise liquidus, electrical resistivity, electro migration, magnetic susceptibility, and densitometry measurements on liquid alloys. Emphasis is placed on liquid alloys of metals that do not form solid intermetallic compounds. Liquidus curve measurements of a number of solutes in liquid Bi and Hg have been made. Quantitative electro-migration data have been obtained on Cr-Bi and Ag-Bi alloys. Apparatus for magnetic susceptibility measurements is being constructed; other measurements are currently underway.

Knowledge of the mechanism of reactions between solid and liquid metals is a major goal. Kinetic measurements and thermodynamic studies of the influence of non-metallic impurities (C, N, O) on the reactions between solid and liquid metals are being planned. These will include studies of interactions of refractory metals with liquid Na at temperatures of 1000-1200°C.

B. Radiation Effects on Metals

1. Fundamental Study of Neutron Irradiation on the Mechanical Properties of Iron and Other BCC Metals
J. Chow and J. S. Bryner

The objectives of this study are to determine the mechanism of radiation hardening and to establish its contribution to the embrittlement of bcc metals. The initial phase of this work will be on high purity iron and iron alloyed with carbon; chromium; nickel; manganese; carbon and chromium; carbon and nickel; and carbon and manganese. Work on other bcc metals is being initiated.

Tensile tests at temperatures ranging from ambient to that of liquid helium are being made on unirradiated and irradiated specimens. Variables such as exposures, irradiation temperatures, thermal annealing temperatures, and grain size are being studied. The effects of irradiation on the dislocation arrangement in pure iron and its alloy is being studied by transmission electron microscopy. Experiments to study the slip traces in polycrystalline and single crystals of irradiated iron at room temperature and near the transition temperature is being initiated.

2. Interaction of Energetic Particles with Metals and Compounds

J. J. Kelsch

The techniques of electron microscopy and electron diffraction are being applied to the study of the physical changes produced in solids by the energy transfer from highly energetic particles >1 mev. The passage of these energetic particles through films produces tracks when the films are of proper thickness.

The origin of specific fission events has been demonstrated in Pt. The vaporization phenomenon begins at the origin i.e. there is no gap at the center of such an event as there is when fission occurs in a photographic emulsion. The effects of both the light and heavy fragments are to be seen in metals of high atomic number. Fission fragment damage has been demonstrated in metals (Al and Ta) in regions whose thickness exceeds 1000Å.

The passage of α particles and tritons of an average energy of 2.5 mev produces tracks in thin films of Li^6F which have been exposed to thermal neutrons to initiate the $Li^6(n,\alpha)H^3$ reaction. This is of interest because of the very low energy of the resultant "particles" compared to fission fragments. An attempt to evaluate damage thresholds as a function of effective Z, and the energy of the moving particle is underway.

An intensive study of film thickness determinations in the 10-500Å range is continuing to improve the quantitative aspects of this research.

3. Diffusion Studies in Ceramic Materials

A. Auskern

This program is concerned with the study and elucidation of diffusion mechanisms of gases in solids. A series of experiments has been completed on the diffusion of xenon-133 from lightly irradiated uranium carbide powder. Another series of experiments is starting on the diffusion of xenon-133 from zirconium carbide powder.

The diffusion experiments with uranium carbide powder have shown that, for the most part, the release of xenon from UC is in accordance with bulk diffusion kinetics. There is in addition, to the bulk diffusion release, lesser initial release of gas the amount of which is roughly proportional to the surface area of the powder. The activation energy for bulk diffusion is about 85,000 cal/mole and the diffusion coefficient for Xe in UC in the temperature range 1000° - 1400°C can be represented by the equation $D = 2.1 \times 10^{-5} \exp -85{,}000/RT$. The activation energy for the initial release appears to be variable, increasing as more and more of the initial gas is released.

Diffusion experiments in zirconium carbide will commence as soon as fabrication of samples is completed. ZrC with variable C content is being prepared by the reaction of ZrO_2 and carbon black.

C. Graphite Studies

1. Interaction of Graphite with its Lamellar Compounds

S. Aronson

A kinetic study of the reactions between graphite and substances with which it forms lamellar compounds has been undertaken. These substances are able to penetrate between the layers of the graphite structure and form compounds of variable compostion. Information will be obtained on the mechanisms of penetration of these substances into graphite and on the manner in which these substances move between the graphitic layers.

The system graphite-bromine is currently under study. Two lines of investigation are being followed. Rates of formation of graphite-bromine compounds are being measured by weight changes in a quartz spring balance system. Rates of exchange of normal and radioactive bromine in graphite-bromine compounds are also being studied. The data obtained to date indicate that bromine penetrates the graphite lattice as part of a graphite-bromine phase of fixed compostion rather than by the diffusion of individual bromine atoms or molecules. The mobility of bromine in graphite-bromine compounds at room temperature is very great. This is evidenced by the rapid exchange of normal and radioactive bromine in these compounds.

A study of the reactions of graphite with other substances, such as the alkali metals, is under consideration. The information obtained from studying these various compounds should throw light on the nature of the interactions between the interstitial species and the graphitic planes.

2. Electrical Properties of Irradiated Graphite

S. Aronson

The electrical properties of irradiated and periodically annealed graphite are under investigation. Irradiated and periodically annealed reactor grade graphite has been found to have interesting and unusual growth and recovery properties. A study of these properties has helped clarify the nature of radiation damage in graphite. In a similar manner, a comparison of the electrical properties of continuously irradiated graphite with periodically annealed graphite should yield useful information regarding the fundamental nature of the electrical changes in irradiated graphite.

Measurements of the electrical conductivity, Hall coefficient, and magnetoresistance are being made on reactor grade graphite which is irradiated at temperatures of 30-60 °C and is annealed at regular intervals up to temperatures of 350 °C. The data so far obtained indicate that damage to the electrical properties caused by irradiation can be completely arrested by the application of periodic annealing techniques. It has, further, been observed that much of the recovery of electrical

properties during heat treatment is not directly associated with the annealing of interstitial complexes. The accumulation of further information on the electrical properties of periodically annealed graphite should yield quantitative information on the nature of the electrical changes in irradiated graphite and on the relationship between changes in the electrical properties and other properties of graphite.

3. Radiation Damage of Graphite
D. G. Schweitzer

The program at BNL is designed to understand the fundamental aspects of radiation damage and recovery in graphite. The number, nature and kinetics of the interstitials formed during the radiation process and their ultimate removal by annealing are being studied.

The program consists of dimensional, stored energy, lattice parameter, porosity and oxidation measurements on graphites that have been subjected to continuous irradiation and periodic irradiations and annealing.

Results to date include an experimental determination of the activation energy for annealing single interstitials in graphite and the absolute rate of formation of displaced atoms in neutron irradiated graphites. The rate of growth of graphite and its dimensional recovery after an annealing operation can be predicted. In addition, dimensional stability can be achieved in irradiated sraphites by a proper combination of irradiations and appropriate periodic annealing temperatures.

A series of reactions have been postulated for the formation and removal of radiation damage in graphite. The model can account for observed stored energy releases and distribution, contraction during early stages of reirradiation, reverse stored energy and C-axis annealing effects, and dimensional stability of heavily damaged graphites.

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Contractor:	Brookhaven National Laboratory, Upton, Long Island, New York
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Contract Title:	BASIC RESEARCH IN THE SOLID STATE DIVISION
Investigators:	G. J. Dienes, G. H. Vineyard and staff

Scope of Work: A. Radiation Effects

1. Optical, Ultrasonic and Magnetic Resonance Studies of Insulators
P. W. Levy, P. Townsend, F. Agullo-Lopez, and C. W. Kocher

A study of the formation and annealing of the color centers in natural quartz is nearing completion. For the first time the absorption spectra have been successfully resolved into the individual component bands, which are non-Gaussian and non-symmetric. This resolution is essential for a detailed interpretation of the annealing steps. One of the annealing steps, that near 240°C in gamma-irradiated quartz, is particularly interesting since it correlates with "peak" in the ultrasonic attenuation obtained when irradiated quartz is heated. Since it is unlikely that any atomic motion is involved in the production or disappearance (on heating) of the coloration produced by gamma-rays alone, these effects most likely involve the motion of electrons and holes. Thus the large ultrasonic attenuation peak observed when the irradiated quartz is heated must be electronic in origin.

Research on irradiated insulating crystals with electron spin resonance techniques is beginning to yield important information on two systems, Al_2O_3 and NaN_3. Electron spin resonances in Al_2O_3 have been induced by ultraviolet, gamma-ray, reactor and high energy electron irradiations. Ultraviolet and gamma-ray irradiations produce the same resonance absorption line while reactor and 1.8 Mev electron irradiations produce different centers. It appears that the electron irradiation causes the displacement of only one atom whereas the reactor irradiation causes more complicated displacements. Gamma-ray irradiation of potassium azide crystals at 77°K creates several paramagnetic defects in addition to the N_4^- molecule-ion previously reported. One of these defects has been identified by its fine and hyperfine structure as a trapped nitrogen atom. Another of the radiation-induced defects has been classified as an N_2^- molecule ion. The trapped nitrogen atoms and the N_2^- molecule ions decrease rapidly upon warming, but the N_4^- is observed to grow in intensity. At room temperature the N_4^- decays with a half-life of about 16 hours.

Photoconductivity measurements represent another important experimental technique for studying insulating crystals. The first extensive measurements with the recently completed photoconductivity apparatus are being done on the radiation induced changes in the photoconductivity of TiO_2. New photoconductive peaks have been observed at 6200 and 5500A which can be populated with ultra-violet light corresponding to the hand gap. The photo current (I) at each peak can be expressed as a function of light intensity (L) by the relation $I = \text{constant} \times L^n$. When exposed to gamma-ray or reactor irradiations the exponent n is altered. The dark current is also changed (by factors of 10 to 1000) by irradiation as well as by oxidation and reduction.

2. Effect of Irradiation on Solid-State Reactions
D. T. Keating, A. C. Damask, F. E. Fujita, and R. A. Arndt

The study of solid state reactions controlled by diffusion and/or nucleation is continuing. Recent experiments have clarified considerably the role of radiation in influencing the kinetics of the disappearance of carbon from solution in iron. Measurements of the rate of decay of the internal friction peak in quenched iron-carbon after a 12 day low temperature irradiation show that the carbon disappears from solid solution over a thousand times faster than in unirradiated iron. This process obeys second order kinetics with an activation energy of 19.8 Kcal/mole, the activation energy for the diffusion of carbon in iron. Calculations indicate that not enough extra precipitation nuclei could have been created by these irradiation doses to cause such an extremely rapid disappearance of the carbon from solution. Electron microscope observation of irradiated samples which have been annealed isochronally up to 100°C reveals no precipitate particles, although this time and temperature is sufficient to complete the decay of both the internal friction peak and the electrical resistivity of specimens irradiated at low temperature. It is concluded that the carbon is being trapped by the vacancies or the interstitials produced by the irradiation and that low temperature irradiation retards the formation of carbon precipitation.

3. Chemical Effects of Irradiation
P. W. Levy and J. Jach

The basic study of radiation effects in easily decomposable materials is continuing. The investigation of the effect of gamma-ray and reactor irradiations on the subsequent thermal decomposition of sodium bromate has been completed. The decomposition is accelerated in a way that suggests that irradiation has enhanced the melting which occurs prior to decomposition. Lead azide as also been studied; the radiation effects on the kinetics of decomposition are extremely marked in this case. The overall rate increased by a factor of 10, the activation energy decreased from 35 to 25 Kc/m, and the pre-exponential factor was reduced by about a factor of 10.

4. Theoretical Calculations
G. J. Dienes, G. H. Vineyard, A. C. Damask, and B. Mozer

a. Radiation Damage Events Machine calculations of radiation damage events in a model which simulates metallic copper have been applied to thermal spike models of radiation damage. Immediately after the most violent stages of a displacement event individual atoms appear to have agitations sufficiently

chaotic to constitute thermal energy. By averaging the kinetic energy of an atom over a time somewhat longer than one Debye period, an effective temperature T can be attributed to that atom. Very drastic heating is observed at short times. The temperature distribution at this time is far from uniform, and there is strong correlation between very hot spots and collision chains. As the event is followed one finds a certain overall resemblance to cooling according to classical laws of heat conduction but with a thermal diffusivity about an order of magnitude higher than values that have commonly been used in thermal spike calculations and the major part of the cooling occurs, in these calculations, at least an order of magnitude faster than has usually been supposed. The very ragged distributions of effective temperature, spreading extremely rapidly and according to complex laws, that are revealed in these studies do not inspire confidence in the significance of conventional discussions of thermal spikes.

b. Impurity Effects on Lattice Vibrational Spectra The above computing machine program has also been used to study changes in the vibrational spectra when an impurity is introduced into the copper lattice. Preliminary results have been obtained for the frequency of a defect mode of vibration for such a simple defect. The frequency of this defect mode has been determined as a function of the mass ratio of the impurity atom to the copper atom. The average displacement from equilibrium of the impurity atom for a given initial velocity has also been obtained as a function of the mass ratio. These latter results are of theoretical interest and useful for interpretation of recent Mossbauer experiments and cold neutron inelastic scattering experiments.

c. Point Defect Annealing Point defects tend to anneal out of any crystal that contains a higher than thermodynamic concentration of defects. It is also known that single point defects can cluster or become attached to impurity atoms. An extensive theoretical study of annealing processes is in progress at Brookhaven based on the isolation and combination of simple kinetic steps. When analytic solutions could not be found, computer solutions have been used to obtain useful approximations and their regions of validity. The following kinetic processes have been investigated so far:

1. Annealing of vacancies and divacancies in pure metals

2. Annealing of vacancies in impure metals.

3. Vacancy-interstitial annihilation with
   a. interstitial migration to sinks,
   b. impurity-interstitial trapping,
   c. diinterstitial formation.

B. Neutron Diffraction Research

The neutron diffraction program continues to be concerned mainly with structural studies on magnetic and ferroelectric crystals. Some studies are also in progress in which crystal structure is of secondary importance. These studies are directed at some fundamental questions in the theory of magnetism, the theory of the liquid state, and the character of crystal transitions.

1. Studies of Magnetic Materials

R. Nathans, B. C. Frazer, H. Alperin, S. J. Pickart, and C. W. Kocher

The emphasis in the magnetic electron density studies has shifted somewhat away from metallic materials to inorganic compounds partly as a result of the lack of suitable single crystal specimens, but also because of the possibility of more direct interpretations of the spin-density maps. Of particular interest is the change in the spatial distributions of the unpaired electrons in Fe^{3+}, Mn^{2+} and Ni^{2+} from the free atom state to one in which they are interacting with their surroundings in a solid. For example, an extensive series of measurements carried out on NiO has not only demonstrated that the magnetic electrons are significantly contracted toward the nucleus over that calculated for the free atom, but in addition they show that the overall moment derived from the neutron scattering is approximately 20 percent lower than expected on the basis of g value for the Ni^{2+} atoms. Such differences could be explained by strong covalent coupling between the Ni^{2+} atoms and their surrounding oxygen atoms.

Recently, there has been a good deal of interest in alloys of the iron group elements with platinum, palladium, and rhodium. Polarized neutron techniques have been used to establish the division of the total moment between the constituent elements and to determine the radial extension of the induced unpaired electrons on the atoms of the non-transition elements. In Pd_3Fe, Pt_3Mn, and RhFe a ferromagnetic arrangement is found, whereas in Pt_3Cr there is a ferrimagnetic grouping of the Pt and Cr atoms. The largest induced moment occurs in RhFe with 1.1μ on the rhodium and 3.1μ on the iron atoms. This alloy is of special interest since it is the first case among the iron alloys where the hyperfine field at the iron nucleus, as determined by Mössbauer experiments, is not proportional to the intrinsic moment on the iron atoms. This effect may be related to the fact that the unpaired electrons on the rhodium atoms are significantly more spread out than the 3d electrons in the iron group series.

The magnetic structures of several alloys of the AB_2 type have been studied. The alloys have Laves type structures and heretofore little had been known about their magnetic behavior. $TiFe_2$ and $ZrFe_2$ were found to be ferromagnetic while $ZrCo_2$ has an antiparallel spin arrangement. The most interesting of these alloys is $TiFe_2$. No moment is found on the Ti atoms, while the Fe atoms, located on two non-equivalent sites, have room temperature moments of 0.2 ± 0.05 and $0.1 \pm 0.05 \mu_B$. The Mössbauer pattern of $TiFe_2$, taken together with these neutron results, demonstrates nicely the linear relation between the magnetic field at the iron nucleus and the intrinsic iron moment.

2. Studies of Non-Magnetic Solids

G. J. Dienes, B. C. Frazer, H. Danner, D. T. Keating, P. J. Brown, H. Boutin, and I. Almodovar

A cold neutron inelastic scattering experiment on nickel-palladium alloys has demonstrated the existence of a simple defect mode of vibration arising from nickel impurities in a palladium lattice. The frequency of the defect mode of vibration is about 1.1 times the maximum frequency expected for pure palladium lattice. The effects of concentration broadening on the defect mode was not observable in the experiment because of poor instrumental resolution.

A study has been started on the inelastic scattering of cold neutrons by liquid hydrogen halides. So far work has been concentrated on liquid HBr. While further measurements must be made on this compound, the results at this stage indicate that very nearly free rotation occurs. It will be of interest to see how the results change on going to the more highly electronegative Cl^- and F^- ions where a much stronger tendency for intermolecular coupling is expected because of hydrogen bond formation.

A neutron diffraction study of gamma- and X-ray irradiated Rochelle salt has been completed. The prevailing view has been that the marked changes in ferroelectric properties with irradiation originate in macrostructural effects, that is, unrelated to the crystal structure. Neutron diffraction and optical studies have shown that important structural changes do occur, although domain mobility must also be considered. The results suggest that there are two basic processes involved when the ferroelectric phase is irradiated: one related intrinsically to the crystal chemical peculiarities of Rochelle salt, and the other to domain pinning. The competition between these processes leads to locked monoclinic domains, stable even at temperatures outside of the normally ferroelectric range. On the other hand, when crystals are irradiated outside the ferroelectric range the crystal structure effects dominate. After sufficient dosage, such a crystal will remain orthorhombic and non-ferroelectric at all temperatures.

Recent Publications:

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Contractor: California, University of, Lawrence Radiation Laboratory, Berkeley, California

Contract Number:

Present Contract Term: July 1, 1962 through June 30, 1963 (Fiscal year 1963)

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Contract Title: BASIC RESEARCH IN THE INORGANIC MATERIALS RESEARCH DIVISION

Investigators: A. W. Searcy, Deputy Director

Scope of Work: A. Mechanical Properties of Metals and Alloys

1. Rate Controlling Deformation Mechanism
J. E. Dorn

The series of investigations described herein are directed toward a better understanding of the atomistic basis for the mechanical behavior of metals and alloys. The principal theoretical tool for this understanding is dislocation theory. Although some progress has been made, both theoretically and experimentally, much yet remains to be done to develop this area of science to an effective degree of maturity.

Dislocation behavior and consequently the mechanical properties of metals and alloys depend on crystal structure, energies of lattice imperfections, electronic energies, solution theory, diffusion, short-range order, long-range order, kinetics of relations, etc. In fact, practically every basic concept of the physics and chemistry of alloys is involved influencing the mechanical behavior of alloy systems. In order to identify how these factors are significant in determining the mechanical properties of metals and alloys, the following investigations were instituted:

(1) An investigation of the dislocation mechanisms associated with plastic deformation, ductility and fracturing in intermetallic compounds.

(2) An investigation of the effect of the strain rate on the concentration of vacancies in metals at elevated temperatures.

(3) An investigation to identify that dislocation process among the host of possible dislocation processes, which controls the strain rate over specified ranges of temperature and stress in magnesium and its alpha solid solutions.

(4) An investigation to determine the details of the dislocation processes responsible for deformation in face-centered cubic metals and their alloys.

2. Effects of Dispersed Phases on Properties of Metals and Alloys
L. Himmel

This study is concerned with the influence which finely dispersed particles of a second phase exert on the properties of metals and alloys. Efforts are being made to establish the manner in which the presence of the dispersed phase modifies the deformation behavior of the matrix and its subsequent response to annealing, i.e., its recovery and recrystallization behavior. The variety of techniques, including transmission electron microscopy, are being used in order to obtain information concerning the interactions between the dispersed particles or clusters and other crystal defects such as vacancies and dislocations. The materials under investigation consist of oxide particles of the order 10Å to 100Å in diameter dispersed in a silver or copper matrix; these materials are prepared by the internal oxidation of dilute solid solution alloys. For comparison purposes, the properties of the unoxidiozed alloys are also being studied.

3. Theoretical and Experimental Properties of Materials
E. R. Parker

Research in progress has been extended to include studies of the strengthening mechanisms in complex alloy systems. One of the main objectives is to obtain an understanding of strengthening processes in such systems. The strongest known type of microstructure, namely martensite, has been selected for the current experimental program. Although the martensite reaction is the most potent strengthening process known to metallurgists, the reason for the high strength thereby produced is not understood.

The starting material used in our case is large single crystals of austenite (rather than the commonly used polycrystalline austenite). Very long martensite needles (about an inch) have been produced and we have found the spread in temperatures between the beginning and end of the austenite to martensite transformation is highly structure sensitive.

The latest results in the ductile ceramic work have been encouraging in that, for the first time, some ductility has been obtained with fine grained lithium fluoride. Elongations in tension teses, ranging from 0.3 to 0.7 percent, have been obtained. Although these are small values, the results prove beyond a doubt that room temperature ductility is possible in such materials. The reason for the ductility is that cross-slip, absent in single crystals, occurs near grain boundaries in polycrystalline material.

4. Relationship Between Structure and Properties of Crystalline Materials
G. Thomas

This study is concerned with the relationship between the microstructure of materials and their properties. The principal research method is transmission electron microscopy allied with other techniques. The work is at present aimed towards mechanical properties, but this will be extended in the near future to include physical properties, e.g., superconductivity. We have also initiated work on the problems of stress-corrosion cracking.

Since mechanical properties depend on the nature and distribution of defects and second phases, many of which cannot be seen without using electron microsocpe techniques, the basic areas of research include correlation of defect structure and plastic flow in pure metals and ceramics. A program on body-centered cubic (BCC) metals is currently underway with niobium and will be extended to include work on BCC alloys. Grain size effects in body-centered cubic and face-centered cubic metals are also being studied. In addition to normal modes of deformation, work is now being done on the structure of explosively deformed metals. Additional work will include studies of vacancies in metals and alloys.

5. Influence of Crystal Imperfections on Mechanical Studies
J. Washburn

The research is directed toward a better understanding of the complex relationships between physical and mechanical properties and structural imperfections in crystalline materials.

Particular emphasis is being placed on an attempt to correlate changes in properties such as specific volume, electrical conductivity, small angle x-ray scattering, plastic flow stress, ductility and mode of fracture with direct observations of defects by means of transmission electron microscopy. Many of the important types of crystal defect can be directly observed at useful magnifications of 100,000 X by this technique. These include dislocation lines, stacking faults, small angle boundaries, and second phase precipitates.

Some specific areas now under study include:

(1) Effect of crystal structure, stacking fault energy and grain size on the maximum hardening that can be achieved by cold work.

(2) A study of the mechanism of vacancy clustering to form prismatic dislocation loops in quenched copper crystals.

(3) The mechanism of dislocation multiplication strain hardening and crack nucleation in face-centered cubic and body-centered cubic metals.

(4) Relationship between plastic deformation and fracture in magnesium oxide.

B. Properties of Ceramics

1. Ceramic Systems: Mechanical Behavior of Multiphase Systems , Internal Strain
R. M. Fulrath

This project is concerned with an investigation of the factors which influence the mechanical properties of polycrystalline single phase and polycrystalline multiphase inorganic non-metallics. The following topics are under study:

(1) The effect of internal stress and interfacial bonding on the mechanical properties of multiphase ceramics.

(2) The nature of grain and interfacial boundaries in ceramics, and their influence on gas permeation under thermal and mechanical stress.

(3) The kinetics and mode of crystallization of Al_2O_3.

(4) The dynamic measurement of strain energy, associated with internal stresses, and reaction heats by differential calorimetry.

2. Ceramic Systems: High Temperature Reactions
A. W. Searcy

The principal objectives of the current programs are to elucidate the equilibra and kinetics for solid-gas reactions at high temperatures. Primary emphasis is placed on experimental and theoretical study of evaporation reactions at solid-gas interfaces.

Currently under investigation are the kinetics and thermodynamics of evaporation of zinc oxide, stannic oxide, indium sulfide, gallium nitride, aluminum phosphate and the reaction of tungsten at very high temperatures and low pressures with oxygen and nitric oxide.

Theoretical development and analysis of models for predicting activation energies for self diffusion in metals and of shapes and stabilities of gas molecules of possible high temperature importance are also undertaken.

3. Ceramic Systems: Mechanical Behavior of Microstructures, Solid State Reactions and Glass Metal Interfaces
J. A. Pask

The deformation of single crystals of several ionic compounds is being determined with orientation, stress, temperature and time as parameters and analyzed on the basis of dislocation theory. The resulting knowledge is being applied to the understanding of the behavior of polycrystalline samples under the same conditions. The ultimate objective is to develop quantitative relationships of the dependence of mechanical behavior of ceramic materials on their microstructure.

Mechanisms and kinetics of solid state reactions and inversions are being studied. Particular interest is being placed on the effect of geometric factors; thus, work with single crystals, polycrystals, and powders is included. The ultimate objective is to translate this knowledge to a better understanding of sintering mechanisms and the development of desirable microstructures.

Fundamental studies are being followed to determine the conditions under which a chemical bond is developed at a glass-metal interface. Nature of interfaces and melting phenomena are being explored. Such factors are particularly important in the development of microstructures involving multiphase systems.

C. Thermodynamics

1. Thermodynamic Functions for the Metallic State

Ralph Hultgren

Critical evaluations of metallic thermodynamic systems have continued as in past years. It is hoped that this work will be completed to be published in book form at the end of summer, 1962, under the sponsorship of the Lawrence Radiation Laboratory of the Atomic Energy Commission. The following systems were completed, multilithed, and distributed since May 1, 1961:

Cs, Fe(revised), Re, Rh, Ru, Sn(revised), U, V, Y, Ag-Pb, Ag-Sb, Ag-Zn, Al-Ca, Al-Ce, Al-Co, Al-Cr, Al-Cu, Al-Mn, Au-Ni(revised), Au-Sn, Ba-Pb, Ba-Sb, Ba-Sn, C-Fe, Cd-Hg, Co-Sb, Cu-Mn, Cu-Ni(revised), Ga-Li, In-Sb, In-Sn, Li-Pb, Li-Sb, Li-Sn, Li-Tl, Mg-Sn, Mg-Tl, Na-Tl.

Recent Publications:

G. Saada, "On the Stability of Quenched Dislocation Loops in Aluminum, Acta. Met. 10, No. 10, (1962) pp. 985-986.

R. L. Nolder and J. E. Dorn, "Activation Energies and Volumes for the Propagation of Luder's Bands," The American Soc. for Metals Transactions Quarterly 55, No. 3, (1962) pp. 505-517.

S. K. Mitra and J. E. Dorn, "On the Nature of Strain Hardening in Face-Centered Cubic Metals," Trans. of Met. Soc. of AIME 224. (1962) pp. 1062-1071.

J. E. Dorn, "Thermodynamics of Stacking Faults in Binary Alloys," UCRL-10487, Sept. 30, 1962. Acta Met. 11, No. 3 (1963) pp. 218-219.

N. A. Jaffe and J. E. Dorn, "Effect of Stress on the Creep Rate of High Purity Aluminum in the Cross-Slip Region," Trans. Met. Soc. AIME 224, (1962) pp. 1167-1172.

Contractor:	Hanford Atomic Products Operation, General Electric Company, Richland, Washington
Contract Number:	AT(45-1)-1350
Present Contract Term:	November, 1962 - June 30, 1963
Cost to AEC:	FY-1963 $85,000 (Includes $5,000 Equipment)
Contract Title:	PLUTONIUM PHYSICAL METALLURGY RESEARCH
Investigators:	J. J. Cadwell, I. D. Thomas, R. D. Nelson, G. E. Miller, F. E. Bowman

Scope of Work:

The objective of this study is the determination of some of the basic physical metallurgical properties of high purity plutonium. Initial studies will involve mechanisms of phase transformation, mechanisms of deformation and fracture, work hardening, recovery, recrystallization and grain growth. A variety of functional tests and measurements, including optical and electron metallography, X-ray diffraction, mechanical deformation, thermal-gravimetry, and calorimetry, are being or will be utilized on "pure" plutonium and phase stabilized plutonium alloys. This will provide information on deformation modes operable in the various allotropic modifications of plutonium, micro-crack initiation and propagation, mechanisms of phase transformation, work hardening, recrystallization, and grain growth.

Progress toward a number of the program objectives will be greatly accelerated if single crystals, pseudo-single crystals, or at least large grained samples can be obtained. Initial attempts will be made to grow single crystal aluminum stabilized delta plutonium samples. Concurrently, large grained alpha plutonium will be formed and preliminary studies on growth of single crystal or pseudo-single crystal alpha will be attempted.

It is expected that progress in the initial phases of this program coupled with results from related programs will influence the specific details of future studies.

Contractor:	Hanford Atomic Products Operation, General Electric Company, Richland, Washington
Contract Number:	AT(45-1)-1350
Present Contract Term:	October, 1957 - June 30, 1963
Cost to AEC:	FY-1958 - FY-1962 $471,470 (Includes $58,418 Equipment) FY-1963 $140,000 (Includes $12,000 Equipment)
Contract Title:	RADIATION EFFECTS ON METALS
Investigators:	J. J. Cadwell, I. D. Thomas, T. K. Bierlein, B. Mastel, H. E. Kissinger, J. J. Laidler

Scope of Work:

The objective of this study is to determine how irradiation affects the properties of metals, how impurities perturb the damage state, and how thermally activated recovery processes operate.

A variety of functional tests and measurements, including transmission electron microscopy, X-ray diffraction, metallography, mechanical deformation, electrical resistivity, and stored energy release, are being utilized on several "pure" metals to provide information on the damage configuration of metals subjected to neutron bombardment, fission fragment bombardment, mechanical working, thermal treatment, and/or quenching.

After neutron irradiation at 40 C to 10^{19} nvt (E>1 Mev) molybdenum specimens contain clustered defects in the form of dark spots, <75 A in diameter. In molybdenum containing >100 ppm carbon an additional defect forms, namely, clearly resolved loops, also <75 A in diameter. Post-irradiation annealing up to 750 C results in no change in the size of the spot defects, a decrease in the number of spot defects per unit volume, an increase in the size of the loops (maximum diameter ~500 A), and an increase and subsequent decrease in the number of loops per unit volume. X-ray diffraction analysis has revealed that the lattice parameter and the {400} half width increases with irradiation, the increase being greatest the higher the carbon content. Decrease in lattice parameter and line width during post-irradiation annealing is also greatest the higher the carbon content. Single crystal molybdenum specimens deform by fine slip in <111> on planes for which the resolved stress is highest, and alternation between two <111> has been observed during tensile deformation tests. No change in deformation processes due to carbon

content or to irradiation has been detected. However, coarse slip rather than fine slip occurs in all irradiated specimens tested.

Major contributions to the field of radiation damage on aluminum and other metals have resulted from this program (see publications appended). Studies are being expanded to include additional parameters, such as irradiation temperature and crystal structure.

Recent Publications:

T. K. Bierlein and B. Mastel, "Defect Structures Observed in Neutron Bombarded Aluminum," Jour. of Applied Physics, 33, (1962) p. 2873.

T. K. Bierlein and B. Mastel, "Fission-Induced Vaporization of UO_2 from a Source and Subsequent Condensation on Collectors Exposed to Fission Fragment Bombardment," Jour. of Nuclear Materials, 7, (1962) p. 32.

H. E. Kissinger, "Diffraction Effects from Irradiated Aluminum Single Crystals," Proceedings Eleventh Annual Conference on Application of X-ray Analysis, Denver. Plenum Press, New York (in press).

Contractor:	Union Carbide Nuclear Company, Oak Ridge National Laboratory, Oak Ridge, Tennessee
Contract Number:	W-7405-eng-26
Present Contract Term:	July 1, 1962 through June 30, 1963 (Fiscal year 1963)
Cost to AEC:	$1,203,000
Contract Title:	BASIC RESEARCH IN THE METALLURGY DIVISION
Investigators:	John Frye, Director, Metallurgy Division and staff

Scope of Work: A. Crystal Physics

1. Crystal Growth

G. W. Clark, C. B. Finch, S. D. Fulkerson, and J. J. McBride

This is a program for studying growth processes of crystals of high-temperature materials. A better understanding of growth mechanisms and system parameters is expected to result in an improved ability to grow monocrystals of controlled perfection, composition, and purity. The materials studied are of current fundamental interest or are suited for the testing of concepts. The facilities include most of the major methods of crystal growth and means for evaluating the grown crystals, both in terms of growth mechanisms and quality.

Equipment for crystal growth now in operation includes hydrothermal furnaces, oxy-hydrogen and oxy-acetylene flame fusion furnaces, a direct-current arc plasma torch and a radio-frequency inductively coupled plasma torch, and systems for growth from molten salt solutions. Crystal evaluation is by optical microscopy and x-ray spectroscopy, with assistance from the broad facilities of ORNL.

Crystals of BeO, ThO_2, and CeO_2 have been grown from melts of $Li_2O.2WO_3$, and melts of other compositions are being investigated for growing crystals of interest. Supercritical water and ammonia have been examined as crystallization solvents, and some apparently new compounds have resulted: $Cs_2O.Fe_2O_3.4SiO_2$, $Rb_2O.Fe_2O_3.4SiO_2$, Cs-, Rb-, and K-iron micas. Magnetite crystals have been grown in 0.5 molar lithium tetraborate near 400°C and 12,000 psi. Improvements are being made in the purity and perfection of crystals of KCl and KBr grown from melts of these substances.

B. Physical Metallurgy

1. Theory of Alloying

J. O. Betterton and G. D. Kneip

This group has as its principal interest the determination of the fundamental factors in alloying early transition elements from Groups IV-A, V-A, and VI-A. Continuing investigations of phase diagrams, low-temperature electronic and lattice specific heats, electrical resistivity and magneto-resistivity, magnetothermal effects, the transition temperature of superconductivity, and high-temperature thermodynamic properties by means of vapor pressures are all used to study both the alloying process and electronic structure of metals and alloys. Studies to date have been concerned mostly with zirconium, but in the field of transport properties this work is being extended to high-purity Group V-A and VI-A single crystals.

A number of advances have been made in the study of superconductivity. A tenfold increase in the critical current was obtained in superconducting Nb-Zr alloy by an impurity-dependent heat treatment. Size effect studies showed that the superconducting current in this alloy flows principally near the wire surface. The useful lifetime of a superconducting magnet has been greatly extended by using metallic insulation between the coils.

One of the first high-field (>10,000 gauss) superconducting magnets was built and is being used in measurements of magnetoresistivity. The first measurements on pure single-crystal tungsten indicate that the conduction in tungsten is by equal numbers of electrons and holes.

2. Relation of Properties to Structure of Metals

C. J. McHargue, R. E. Reed, and R. A. Vandermeer

The purpose of this program is to study the principles dictating atom rearrangements brought about by thermal treatment, mechanical deformation, phase transformations, and irradiation.

Theoretical expressions for impurity-controlled and impurity-independent grain-boundary migration during recrystallization have been developed, have been confirmed by data on zone-refined aluminum containing low contents of copper, and are being applied to aluminum with other additives.

Mechanical twins have been found and crystallographically characterized in electron-beam-melted niobium deformed by high speed impact at room temperature and by slow or fast compression at -196°C. The addition of interstitial elements, especially carbon, inhibited twinning and promoted cleavage cracking in niobium. Transmission electron micrography has revealed networks of dislocaton in rolled niobium, and the interaction of dislocations with interstitial impurities in niobium is being studied. Stacking fault probabilities have been determined for thorium, cerium, and nickel.

Prior reactor irradiation of copper has been found to change the texture of preferred orientation produced during cold rolling. Fiber textures in rods are being determined, analyzed, and correlated with other properties.

3. Metallurgy of Superconducting Materials
M. L. Picklesimer, E. E. Barton, and G. R. Love

Certain alloys which exhibit superconductivity have been found to retain their superconductivity in high magnetic field strengths. This makes it possible to build high-field superconducting magnets with negligible power consumption. Such magnets are useful in many areas of physical research and are potentially of great importance in the thermonuclear program. Known high-field superconductors exist in the niobium-tin and niobium-zirconium systems, and others are expected in the systems technetium-zirconium, technetium-molybdenum, and technetium-niobium. Phase equilibria and the effects of heat treatments, morphology, impurity content, composition, and stress state on superconducting properties are being studied for these five stystems.

A number of new intermetallic phases have been found in the niobium-tin system. Transformation kinetic studies have been made on zirconium-niobium alloys in the composition range of interest. Purified technetium and some of its alloys with zirconium and molybdenum have been cast and forged for the first time, and investigation of ther structures has been started.

4. Deformation in Crystalline Solids
R. O. Williams, J. A. Wheeler, and R. Arsenault

Topics under current investigation include measurements of the stored energy of deformation in metals and alloys and the kinetics of the release of this energy during recovery and recrystallization.

Most progress has been made using a newly constructed calorimeter to measure energy stored during deformation. The procedure is as follows: A tensile sample is deformed isothermally in a bath of a suitable refrigerant such as a "Freon," care being exercised to ensure adequate thermal isolation. The heat generated within the sample is removed by the evaporation of the refrigerant giving a measured volume of gas which can be converted into energy by means of the heat of evaporation. The energy input is given as the integral of the stress-strain curve. The stored energy is the difference between the input and the output. The results so far indicate that the present equipment is adequate for those materials which store appreciable energy and which are relatively strong. The equipment is designed to operate between -196 and 25°C.

Stored energy resulting from deformation has been measured on a series of copper-zinc and nickel-aluminum alloys at -196 and -30°C. The rate of energy storage increases with strain for the first 20% elongation. Alloying increases the energy storage more than it does the strength. A reduction in temperature increases significantly the energy stored in pure metals but has only a minor effect on metals with high alloy content. The results are being interpreted in terms of structural changes in the metals, and measurements will be extended to other systems.

C. Ceramics Research

1. Sintering Studies

C. S. Morgan and C. S. Yust

High-temperature materials are often fabricated by sintering of compacted powders. This program is directed toward an understanding of the mechanism of sintering, particularly in thorium oxide.

Several observations indicate that materials having the fluorite (CaF_2) crystal structure, including thoria, sinter by a mechanism which is dominantly plastic flow rather than diffusion. Among these are a very high-temperature dependence in the sintering rate of ThO_2, high dislocation densities at weld necks formed between CaF_2 crystals, inhibition of sintering of compacts of ThO_2 or CaF_2 by heat treatment below the sintering temperature, and decrease during sintering in the grain size near holes in CaF_2.

Maxima and minima have been found in the sintering rates of ThO_2, CaF_2, CeO_2, and Al_2O_3 powder compacts heated at constant rates. The self-diffusion coefficient of thorium in ThO_2 has been measured at several temperatures.

Sintering rate measurements, dislocation observations, and other studies described are being completed and extended to other materials.

D. Structure and Physical Properties of Liquids and Solids

1. Physical Property Studies

D. L. McElroy, W. Fulkerson, and T. G. Kollie

Apparatus is being assembled and tested for measuring over a wide temperature range the thermal conductivity, thermal diffusivity, and total hemispherical emittance of ceramic materials. Effects of stoichiometry, grain size, impurities, porosity, and prior irradiation on these properties are under investigation.

Different apparatus types are needed for measuring thermal conductivity in different temperature ranges. A thermal comparator apparatus requiring relatively small specimens has been operated to 400°C. A radial heat flow apparatus has been developed to eventually measure thermal conductivity up to 1600°C. It has been used successfully up to 1300°C to obtain rather precise measurements of the thermal conductivity of UO_2, and difficulties in the apparatus are being corrected to permit measurement at higher temperatures. Construction has started on a direct-heating apparatus to measure thermal conductivity up to 2200°C.

A fluidized-bed quenching apparatus for measuring thermal diffusivity to 1400°C is being tested on INOR-8. Apparatus for measuring the total hemispherical emittance has been used on specimens of platinum, Nb-1% Zr, and polished and oxidized INOR-8.

2. Spectroscopy of Ionic Media
G. P. Smith, C. R. Boston, and H. W. Joy

This group studies optical, electronic spectra of molten salts directed toward the measurement of ion interactions and the "structure" of melts. Progress is being made along both theoretical and experimental lines. Current research is being made along both theoretical and experimental lines. Current research is concerned with charge-transfer spectra of several types and with spectra of solutions of metals in molten salts. Studies now at an advanced state of investigation are described below.

An internal charge-transfer transition of the nitrate ion is found to change in systematic ways with systematic changes in the cation composition of nitrate melts. A theory pertaining to the observed transition-energy shifts has been developed. The results of theory and measurements indicate elements of quasi-crystalline structure in nitrate melts.

The spectra of solutions of bismuth metal in melts of $BiCl_3$ and $BiBr_3$ show that the solute is partitioned between two species, probably Bi^- and $(Bi_3)^{3-}$. The data fix the partitioning constant and its temperature dependence. These results have a decisive bearing on current debate over the atomistic nature of metal-molten salt solutions of posttransition metals.

A new high-temperature spectrophotometer has been procured, capable of precise measurements above 1000°C.

Progress is being made on developing a code for machine calculation of multi-center wave functions for molecules and molecule ions.

3. Fundamental Research in X-Ray Diffraction
H. L. Yakel, B. S. Borie, and C. J. Sparks

The objective of this program is the use of x-ray diffraction techniques to determine the structure of crystalline materials. A major part of this effort is the determination of atomic positions in new alloys and compounds. To some extent this involves collaboration with the research groups discovering these new materials.

Using diffuse scattering, an unusual short-range structure has been found for the alloy Cu-16 at. % Al in both irradiated and unirradiated samples. An improved LiF monochromator has been designed and built, more than doubling the intensity of monochromatic x-ryas available for diffuse scattering measurements.

A selective broadening has been found in the x-ray diffraction patterns of BeO irradiated to a fast neutron dosage of 1.5×10^{21} nvt. This has been interpreted in terms of interstitial clusters. Investigation of effects of radiation is continuing. High-temperature x-ray diffraction has been used to study the order-disorder transition which takes place in Cu-32.2 at.% Au at 313 to 328°C. An approximate structure has been found for the compounds $AMnO_3$, where A is holmium, erbium, thulium, ytterbium, lutetium, or yttrium.

Structure determinations on new compounds, including $SmScO_3$, $GdScO_3$, Sc_2TiO_5, and $CsFeSi_2O_6$, are continuing.

E. Chemical Properties of Solids

1. Reactions at Metal Surfaces

J. V. Cathcart, R. E. Pawel, and G. F. Peterson

The general purpose of this program is the investigation of the fundamental processes involved in the oxidation of metals. The principal direction of approach is the study of factors affecting the protectiveness of oxide films on metals, particularly the strain in the films.

Studies of the oxidation characteristics of refractory metals such as niobium and tantalum have demonstrated the importance of the mode of diffusion in the oxide film and the oxide-to-metal volume ratio as strain-producing agencies. The application of a variety of methods of study (e.g., electron microscopy, kinetic measurements, x-ray and electron diffraction, and optical metallography) to these systems has revealed the importance of the geometry of the oxide interfaces as a factor in the generation of stresses in oxide films. Oxidation rates measured on single crystals of tantalum show little anisotropy. During early stages of the oxidation of tantalum, surface stresses of about 50,000 psi are observed.

The rate of sulfidation of tantalum is under investigation and it appears to show a maximum in the temperature range 700-800°C. Preliminary studies are under way on the nitridation of tantalum.

Continuing x-ray and optical studies of thin oxide films on single crystals of copper have shown the existence of large strains in the films. These strains appear to have an epitaxial origin, and they induce optical anisotropy in all of the films except those on the (111) and the (100) crystallographic planes where both oxide and metal possess a high degree of rotational symmetry.

Recent Publications:

R. O. Williams, "Stored Energy and Release Kinetics in Lead, Aluminum, Silver, Nickel, Iron, and Zirconium," Trans. Met. Soc. AIME 224, (1962) pp. 719-26.

R. O. Williams and J. A. Wheeler, Jr., "The Stored Energy of Cold Work of Alloys as a Function of Composition and Temperature," J. Metals, 14(9), (1962) p. 708.

C. R. Boston and G. P. Smith, "Spectra of Dilute Solutions of Bismuth Metal in Molten Bismuth Trihalides. I. Evidence for Two Solute Species in the System Bismuth-Bismuth Trichloride," J. Phys. Chem., 66, (1962) p. 1178.

G. P. Smith and C. R. Boston, "Cation-NO_3^- Coordination in Fused Nitrates Studied by Means of Shifts in the UV Spectrum of NO_3^-," Proceedings of the 7th International Conf. on Coordination Chemistry, Stockholm and Uppsala, Sweden, June 25-29, 1962, Almquist and Wiksell, Uppsala. p. 93.

H. W. Joy, "Integrals of Products of Associated Legendre Functions," J. Chem. Phys , 37, (1962) p. 3018.

J. O. Betterton, Jr., et al., "Size Effect and Interstitial Impurities in Nb_3Zr Superconducting Solenoids with Metal Insulation," Superconductors, pp. 61-81, edited by M. Tanenbaum and W. Wright, Interscience Publishers, New York, 1962.

D. S. Easton and J. O. Betterton, Jr., "The Phase Diagram of Zirconium-Gallium," J. Metals, 14, (1962) p. 685.

J. O. Betterton, Jr., and D. S. Easton, "Magnetoresistance and Transverse Voltage, That is Even with Respect to the Field, in Tungsten," Bull. Am. Phys. Soc., 7, (1962) p. 618.

G. D. Kneip, Jr., J. O. Betterton, Jr., and J. O. Scarbrough, "Specific Heats of Zirconium Alloys," Bull. Am. Phys. Soc., 8, (1963) p. 66.

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M. L. Picklesimer and S. T. Sekula, "Superconducting Transition Temperature of Purified Technetium," Phys. Rev. Letters, 9(6), (1962) p. 254.

M. L. Picklesimer, "A Note on Some of the Intermediate Phases in the Nb-Sn System," Appl. Phys. Letters, 1(3), (1962) p. 64.

B. S. Borie, C. J. Sparks, Jr., and J. V. Cathcart, "Epitaxially Induced Strains in Cu_2O Films on Copper Single Crystals - X-Ray Diffraction Effects," Acta. Met., 10, (1962) p. 691.

L. A. Harris, R. A. Potter, and H. L. Yakel, "Preliminary Observations of Mixed Oxide Compounds Containing BeO," Acta. Cryst. 15(6), (1962) p. 615.

H. L. Yakel, "Systematic Multiple Diffraction in Equi-inclination Weissenberg Geometry," Acta. Cryst. 15(11), (1962) p. 1188.

H. L. Yakel, "High Temperature X-Ray Diffraction Study of the Order-Disorder Transition in a Cu-32.2 Atomic Percent Gold Alloy," J. Appl. Phys. 33(8), (1962) p. 2439.

T. G. Godfrey, T. G. Kollie, and D. L. McElroy, "The Thermal Conductivity of INOR-S between 100 and 800°C," Trans. Asm Quart., 55(3), (1962) pp. 759-51.

D. L. McElroy, T. G. Kollie, W. Fulkerson, T. G. Godfrey, and H. W. Godbee, "Thermal Conductivity Measurements at the Oak Ridge National Laboratory," pp. 17-30 in Proceedings of the 2nd Conf. on Thermal Conductivity, National Research Council, Oct. 10-12, 1962. (1962).

Contractor:	Union Carbide Nuclear Company, Oak Ridge National Laboratory, Oak Ridge, Tennessee
Contract Number:	W-7405-eng-26
Present Contract Term:	July 1, 1962 through June 30, 1963 (Fiscal year 1963)
Cost to AEC:	$1,860,000
Contract Title:	BASIC RESEARCH IN THE SOLID STATE DIVISION

Investigators: **D. S. Billington, Director; J. H. Crawford, Assistant Director, Solid State Division and staff**

Scope of Work:

This research program is dedicated to securing a basic understanding of radiation damage in solids. Attaining this goal requires a detailed understanding of the interaction of radiation with matter in a quantitative fashion, namely, a knowledge of the number and type of defects introduced by various types of energetic radiation into a wide variety of solids, information which must be gained from experimental measurement. Since, even in the absence of radiation, our knowledge of the modes by which defects influence physical behavior is very inexact, it is necessary to resort to studies that illuminate this interrelationship preparatory to radiation studies. Thus the magnitude of the total task is huge and no simple solution appears readily available. However, it is evident that the area of study called radiation damage has become an important part of solid state and as such holds great promise of aiding substantially in the ultimate understanding of the defects in solids. A brief summary of the progress follows.

A. Theoretical Studies

1. Range Calculations

D. K. Holmes, E. J. Lee, C. Lehman, G. Leibfried

A general program is underway for the study of the process of slowing down of energetic atoms in solid materials. The interesting physical quantities which may be obtained from this study are the vector range of the atoms, the penetration of the atoms along their original directions of motion, and the lateral spread. At the basis of all theoretical studies is the interatomic potential, the form of which must be assumed in the present state of knowledge; however, comparison of the theoretical calculations with pertinent experimental results should give a greatly improved knowledge of such potentials. Considerable effort has been spent in an attempt to calculate ranges analytically; however, while it is possible to compute formally averages of all sorts over the distribution of finally stopped atoms, it is very difficult to make numerical calculations without the benefit of simplifying assumptions. Consequently, another large effort has been expended in Monte-Carlo-type computations using large, high-speed machines, in which the entire slowing-down history of an atom is followed. Two versions of this method are currently in use:

(1) the "random model", in which the lattice is randomized but crystal density is preserved, and (2) the "lattice model", in which the full lattice symmetry is retained. To date, results principally from the random model have been compared with experiment with the objective of finding a suitable interatomic potential. An interesting result from the lattice model has been the discovery of the possibility of long-range channeling of moving atoms through "open" lines in the lattice. The extent of such an effect is now being calculated analytically.

Analytical effort on the general range problem is now concentrated not only on finding rigorously correct expressions for averages of all orders over the final distribution of stopped atoms, but also on discovering appropriate approximation methods, as determined by comparison with the Monte Carlo results. The hard sphere approximation has received particularly close attention and several methods for choosing the hard sphere radius have been tried, namely: (1) the distance of closest approach in a head-on collision, (2) the distance of closest approach in a given trajectory, and (3) the matching of the stopping power. A simple approximating potential has been found which allows the atomic scattering to be calculated analytically and yet gives results agreeing closely with the accurate calculations.

2. Sputtering Theory
M. T. Robinson, C. Lehmann

In connection with experimental sputtering program, considerable attention has been devoted to the theory of sputtering. While all sputtering theory is in a relatively primitive state, it has been possible to understand some of the gross aspects of the experimental results through the use of two ideas:

(1) By considering the "transparency" of the (single) crystal to ions incident on various surfaces, one may account quite well for the orientation dependence of sputtering.

(2) By considering the ejected atoms as resulting from focusing chains initiated within the crystal, one may account for the "spot" pattern of sputtering and obtain rough agreement with the total yield values.

3. Semiconductor Theory
H. C. Schweinler, J. W. Miller

A report has been prepared and issued describing an IBM 7090 program for computing the Fermi level in nonmetals.

In considering the minority carrier lifetime in nonmetallic crystals it is noted that when a flux of charged particles impinges upon a charged capturing center, the capture probability is modified by Coulomb attraction or repulsion. A function which relates the experimentally observed capture probability to an atomic capture probability has been defined and tabulated.

4. Other Theoretical Work

H. C. Schweinler

Some attention has been given to critical simplices in the reduced Brillouin zone. Expecially, the 0-simplices (points) can be written down for the case of a square lattice of points.

Theoretical considerations show that in particular cases interstitial atoms may be observed through their emission of Mossbauer radiation.

An IBM 7090 computer program has been written for calculating the number of primary displaced atoms produced by bombardment with energetic electrons.

B. Radiation Effects in Semiconductors

O. L. Curtis, R. F. Bass, J. C. Pigg, O. E. Schow, M. Chester

The study of radiation effects in semiconductors is used as a means of determining the fundamental nature of defects in solids. Semiconductors are especially useful for this study because of their unique electrical properties and the sensitivity of these properties to crystalline defects. Besides their role in contributing to the fundamental knowledge concerning solid state physics, these studies are of immense practical importance to those who must make use of solid state devices which are exposed to radiation. A variety of materials are used in this program. These include the elemental semiconductors germanium and silicon, and compound semiconductors such as the sulfides of zinc, cadmium, and mercury.

A wide variety of complementary measurements are made. Among these are measurements of transient photoconductivity (this includes measurements of minority carrier lifetime), Hall effect, conductivity, thermoelectric power, and scintillation decay. Equipment is now being prepared for the measurement of dc photoconductivity, and photo-Hall effects. Among the experimental techniques contemplated for future use are: thermal stimulation of trapped carriers, infrared quenching of photoconductivity observation of the dependence of current upon applied voltage using ohmic contacts (space charge effects), and electroluminescence.

C. Radiation Effects in Metals

1. Role of Defects in Surface Reactions

F. W. Young, Jr., L. H. Jenkins, L. D. Lulett, U. Bertocci, and J. R. Savage

A particularly important area of study is the role of defects in determining the course of reactions that take place at metal surfaces. One aspect of this program has been the attempt to characterize the surface of a good metal such as copper. A great deal of attention has been devoted to preparing copper single crystals with a low dislocation density, so that the effects of surface orientation and defect structure on the dissolution process can be properly studied. The role of

current density, solution composition, and orientation of electrode surfaces on the development and growth of etch pits at dislocations is being studied intensively. Etch pit techniques are being used also to study dislocation behavior in deformed copper crystals both in the annealed state and in the irradiated state.

2. Effects of Low Temperature Irradiation
R. R. Coltman, V. R. Klabunde, J. K. Redman, B. Fielder, and D. L. McDonald

One of the most fruitful approaches to investigations of radiation damage has employed low temperature irradiation. The facility in the ORGR that permits irradiation at temperatures as low as $3^{\circ}K$ has been very useful in providing data that can be treated in a quantitative fashion. That is, the temperature of irradiation is low enough to preclude recombination and/or annealing of radiation-produced defects so that appropriate property measurements, such as electrical resistivity, length change, or stored energy, have provided excellent information in regard to the rate of production of defects in a nuclear reactor and the thermal stability of these defects. Recent work has involved a more detailed study of the damage caused by recoils from energetic capture gammas.

3. Internal Friction Studies
D. O. Thompson, and V. K. Pare'

This sensitivity of internal friction and Young's modulus measurements to dislocation pinning makes them a valuable tool in studying radiation effects under reproducible conditions. Recent investigations of neutron-irradiated, high-purity copper single crystals yield evidence for vacancy clustering at dislocations which can be revealed by a suitable change of temperature subsequent to irradiation.

4. Sputtering
A. L. Southern, M. T. Robinson

An increasing interest in the close relationship between sputtering and radiation damage has led to a study of sputtering yields and atom ejection patterns from single-crystal zinc and aluminum after bombardment with 4-kev agron ions.

5. Effects of Irradiation on Superconductivity
S. T. Sekula and W. T. Gerg

We have recently undertaken a study of superconducting metals and alloys. A preliminary study of the superconducting properties of tin during irradiation in the reactor did not show any significant changes. A determination of the transition temperature of technetium has led to a value of $8.22^{\circ}K$. The mechanical properties of Nb-25% Zr are being determined at $300^{\circ}K$, $77^{\circ}K$, and $4.2^{\circ}K$.

6. Fission Track Studies
T. S. Noggle and B. F. Day

The intensive study of fission tracks in UO_2 and thin metal films is continuing. The ability to observe by transmission electron microscopy fission tracks and defects such as dislocations makes this technique most valuable in interpreting radiation effects in UO2 and metals. Replication techniques are being used for studies of surface defects in high-purity copper single crystals.

D. Radiation Effects in Insulating Crystals

J. H. Crawford, Jr., E. Sonder, W. A. Sibley, L. C. Templeton, and R. B. Murray

A number of investigations pertaining to defects in insulators and their production by energetic radiation are in progress. The most important of these from the standpoint of radiation damage is a study of the mechanism of defect production by ionizing radiation.

In ionic crystals and crystals with partially-ionic-binding character, the radiochemical processes which lead to the production of point defects and aggregates of these are not well understood. In highly ionic materials, such as the alkali halides, this mode of defect introduction dominates displacement-type damage in irradiated crystals. The situation near room temperature is further obscured by the extensive structure sensitivity of the radiolysis, a fact which reveals the great importance of purity and perfection of research specimens in such studies.

Investigations include:

1. Color Center Studies

E. Sonder and W. A. Sibley

Studies of the interrelationship between defects responsible for F-centers and M-centers and ultraviolet centers in a wide variety of KCl specimens exposed to γ-rays and Van de Graaff electrons. It has been shown that the relative development of these centers is markedly affected by both crystal purity and the intensity of ionization during irradiation near room temperature. Interpretations of these observations in terms of the influence impurities exert on electronic behavior and quenched-in defect structure are being sought.

2. Magnetic Properties

E. Sonder and L. C. Templeton

Magnetic susceptibility measurements are being employed to characterize color centers in KCl which have not yet been identified. A recent study of the M-center revealed that it is not paramagnetic, thereby confirming the di-F-center model proposed by Van Doorn. This technique will be applied to other centers in alkali halides and other insulating crystals.

3. Radiation Hardening

W. A. Sibley

Hardening of KCl by radiation is being studied. The radiolytic defects impede the motion of dislocations. Details of the hardening mechanism are under investigation. In this connection, dislocations and their interaction with point defects are being further studied in alkali halides by means of light scattering and internal friction techniques.

4. Electron Spin Resonance Investigations
R. A. Weeks

Electron spin resonance investigations of radiolytic and displacement type defects in a variety of insulators, including SiO_2, TiO_2, Al_2O_3, and MgO, are in progress. A combination of ESR and optical studies has led to the identification of the magnetic centers responsible for certain optical absorption bands and to the construction of models for the responsible defects. Such studies will be extended to other materials.

5. Scintillation and Luminescence
R. B. Murray and A. Meyer

The scintillation process in alkali iodides containing thallium has been extensively investigated. Results have shown that quenching of scintillation at low temperatures can be accounted for on the basis of the self-trapping of holes. This suggests that luminescence originating at the thallium ion is due to electron-hole recombination.

Equipment for the investigation of luminescence and thermoluminescence has been constructed. Investigations in these areas will be directed toward an understanding of the role impurities and structural defects play in electro-optical transitions in insulators.

Recent Publications:

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M. J. Smith, "Determination of the Nonstoichiometric Doping Mechanism in Bi_2Se_3," Appl Phys. Letters, 1, (1962) p. 79.

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G. Leibfried, "Calculations of Averages for Primary Recoil Distributions," J. Appl. Phys. 33, (1962) p. 1933.

G. Leibfried and O. S. Oen, "A Simple Approximation for Classical Scattering at Large Angles," J. Appl. Phys. 33, (1962) p. 2257.

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Axel Meyer and R. B. Murray, "Effect of Energetic Secondary Electrons on the Scintillation Process in Alkali Halide Crystals," Phys. Rev. 128, (1962) p. 98.

Mark T. Robinson, "Deduction of Ion Ranges in Solids from Collection Experiments," Appl. Phys. Letters 1, (1962) p. 49.

Mark T. Robinson, D. K. Holmes, and O. S. Oen, "Monte Carlo Calculations of the Ranges of Energetic Atoms in Solids," p. 105 in Le Bombardment Ionique, Centre National de la Recherde Scientifique, Paris, 1962.

A. L. Southern, William R. Willis, and Mark T. Robinson, "Sputtering Experiments with 1- to 5-kev Ar^+ Ions," J. Appl. Phys. 34, (1963) p. 153.

G. Leibfried, "Higher Order Averages of Primary Recoil Distributions," Z. Physik 171, (1962) p. 1.

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F. W. Young, Jr., "Etch Pit Studies of Dislocations in Copper Crystals Deformed by Bending: I Annealed Crystals; II Irradiated Crystals," J.Appl. Phys. 33, (1962) p. 3553.

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J. W. Cleland and R. F. Bass, "Lattice Defect Production in Ge by Photons and by Neutrons," Bull. Am. Phys. Soc. (II) 8, (1963) p. 235.

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R. A. Weeks and E. Lell, "The Effects of Irradiation on Polarization Currents in a Lead Silicate Glass," Bull. Am. Phys. Soc. 8, No. 4 (1963)

J. M. Willians, M. S. Wechsler, and J. H. Barrett, "2nd-Run Phenomenon in Irradiated Cu-15 at.% Al," Bull. Am. Phys. Soc. 8, (1963) p. 196.

PART II

OFFSITE RESEARCH

Contractor: Alabama, University of, University, Alabama

Contract Number: AT(40-1)-3090

Present Contract Term: February 15, 1963 through February 14, 1964

Cost to AEC: $26,705

Contract Title: f-SHELL TRANSITION STUDIES

Investigators: Edward H. Carlson

Scope of Work:

Several topics will be investigated including: Analysis by optical and EPR spectroscopy of transition ion pair and defect spectra, a search for compounds with ordered states (ferro- or antiferromagnetic), and spin-phonon scattering processes.

These studies will be carried out in materials having simple structure, such as doped CaF_2 and MgO and the anhydrous fluorides and chlorides of La, Ce, Pr, Nd and Sm. The study of pair spectra allows one to determine the exchange interactions between transition ions and thus predict the presence and properties of ordered states. The latter will be sought in concentrated materials using susceptibility bridge measurements, and NMR and EPR, and perhaps by specific heat measurements.

The spin-phonon interaction will be studied by heat conduction measurements in doped materials as a function of temperature, doping concentration and magnetic field.

Contractor: Andrews University, Berrien Springs, Michigan

Contract Number: AT(11-1)-972

Present Contract Term: June 1, 1962 through May 31, 1963

Cost to AEC: $9,500

Contract Title: MECHANICAL PROPERTIES OF SEPARATED METALLIC ISOTOPES

Investigators: Donald D. Snyder

Scope of Work:

Continued studies will be made on the effect of isotopic mass on the phase transitions in isotopically enriched lithium. Present studies have been limited to the temperature range of 63°K to 295°K but will be extended to the range 4.2°K to melting point (ca 460°K). More intensive study will be made of the new transition observed at about 140°K as well as the well known one at 77°K. X-ray analysis of the crystal structure will be carried out. It is anticipated that contemplated changes in the apparatus will make it possible to extend the observation to include measurements on oscillation damping in the material. Extension of the program to include isotopically enriched magnesium is planned.

Contractor:	Arizona State University, Tempe, Arizona
Contract Number:	AT(11-1)-715
Present Contract Term:	January 15, 1962 through January 14, 1963
Cost to AEC:	$20,242
Contract Title:	AN INVESTIGATION OF THE OPTICAL AND ELECTRICAL PROPERTIES OF INSULATORS AND SEMICONDUCTORS WHICH HAVE BEEN EXPOSED TO IONIZING RADIATION
Investigators:	B. R. Gossick

Scope of Work:

The electrical resistivity of pile irradiated semiconducting rutile has been investigated, using dense ceramic samples. The resistivity was found to be relatively insensitive to pile irradiation, requiring an integrated flux of around 10^{16} fast neutrons/cm^2 to produce a detectable change in samples with resistivity in the range 1-10 ohm cm at room temperature. The resistivity increases with bombardment, indicating that centers are produced which trap conduction electrons. The percentage change in resistivity induced by bombardment is greater with low resistivity material, indicating a dependence of the formation rate of trapping centers on the concentration of donors (presumably oxygen vacancies). It is proposed to extend these studies to single crystal rutile.

The optical extinction of halide crystals is being studied before and after exposure to x-rays. The bands, associated with metal particles that might be expected to form in the crystal, define that part of the spectrum which is under investigation. The scattering by metal precipitates in NaF, CaF_2 and CsBr crystals will be sought using dark field illumination.

Contractor: Arizona, University of, Tucson, Arizona

Contract Number: AT(11-1)-1040

Present Contract Term: June 15, 1962 through June 14, 1963

Cost to AEC: $11,793

Contract Title: THE FREQUENCY OF ANNEALING TWINS

Investigators: D. J. Murphy

Scope of Work:

Measurements of the activation energy for the movement of a noncoherent annealing twin boundary are being made on coarse grained or single crystal specimens of copper, and a series of copper-rich solid solutions. Attempts will be made to move a coherent annealing twin boundary mechanically, and the necessary mechanical energy determined. Determinations of twin profiles are made to furnish quantitative data on the three-dimensional geometry of annealing twins and help clarify the nature of noncoherent boundaries. Quantitative determinations of solute segregation at annealing twin boundaries are sought through the use of an electron probe x-ray microanalyzer and from electrical resistivity measurements across the boundary. Solute segregation determinations are also made by electrical resistivity measurements by using electrical probes to determine the electrical resistivity across twin boundaries.

Contractor: Arizona, University of, Tucson, Arizona

Contract Number: AT(11-1)-1041.

Present Contract Term: June 1, 1962 through May 31, 1963

Cost to AEC: $47,744

Contract Title: IMPURITY DIFFUSION IN SOLIDS

Investigators: Carl T. Tomizuka

Scope of Work:

The diffusion of impurities in metals is the subject of this research program. The primary objective of the research, utilizing a tracer technique for measurement of rates of diffusion, is to obtain reliable data on impurity diffusion which can be used to test the Lazarus-LeClair screening theory. The research also involves determination of the activation volume for impurity diffusion and study of the effect of pressure on the screening radius. Initial studies are carried out with Cu and Ag as solvents. Subsequent stages of the program may include study of the effect of pressure on diffusion in ionic crystals.

Recent Publications:

C. T. Tomizuka and R. M. Emrick, "Lattice Parameter Correction to Diffusion Coefficients," submitted to Journal of Applied Physics.

J. S. Armijo, J. Steedley and C. T. Tomizuka, "Internal Friction and Self-diffusion in Alpha-brass of 15 at % Zn," submitted to Acta Metallurgica.

Contractor: Arkansas, University of, Fayetteville, Arkansas

Contract Number: AT(40-1)-2096

Present Contract Term: November 1, 1962 through October 31, 1963

Cost to AEC: $27,993

Contract Title: STUDY OF STRUCTURES OF LIQUIDS BY X-RAY DIFFRACTION

Investigators: P. C. Sharrah and R. F. Kruh

Scope of Work:

Structural studies of liquids by x-ray diffraction are made on two main classes of materials: Liquid metals and solutions of complex ions. The former includes the alkali metals and their binary alloys, and amalgams of copper, aluminum, and zinc. In addition, the temperature dependence of the scattering from liquid mercury, zinc, and bismuth is being investigated. The studies of solutions include measurements on water as a function of temperature aqueous solutions of isopolymolybdates, and nonaqueous solutions of transition metal halides. New sample systems will also permit examination of liquefied gases and liquid bromine and iodine.

Recent Publications:

J. I. Petz, R. F. Kruh, G. C. Amstutz, "X-Ray Diffraction Study of Lead Sulfide-Arsenic Sulfide Glasses," J. Chem. Phys. 34, (1961) p. 526.

Y. S. Kim, G. L. Standley, R. F. Kruh, G. T. Clayton, "X-Ray Diffraction Study of Liquid Mercury-Indium Alloys," J. Chem. Phys. 34, (1961) p. 1464.

C. L. Standley, R. F. Kruh, "On the Structure of Ferric Chloride Solutions," J. Chem. Phys. 34, (1961) p. 1450

P. C. Sharrah and R. F. Kruh, "On the Structure of Liquid Metals," Physical Chemistry of Process Metallurgy, Vol. 7, (1961) pp. 419-420.

R. F. Kruh, "Diffraction Studies of the Structure of Liquids," (Accepted for publication in Chemical Reviews.)

R. F. Kruh and C. L. Standley, "An X-Ray Diffraction Study of Aqueous Zinc Chloride Solutions," Inorg. Chem. (to appear in Vol. 1, No. 3).

R. F. Kruh, "Diffraction Studies of the Structure of Liquids," Chem. Reviews, August 1962.

R. F. Kruh and R. M. Lawrence, "X-Ray Studies of Ion Interactions in Solution," (submitted to Inorg. Chem.).

R. F. Kruh, G. T. Clayton, Charles Head, Glen Sandlin, "The Structure of Liquid Mercury," (submitted to Phys. Review).

Contractor: Armour Research Foundation, Chicago, Illinois

Contract Number: AT(11-1)-578, Proj. No. 9

Present Contract Term: February 15, 1962 through February 14, 1963

Cost to AEC: $83,530

Contract Title: MAGNETIC PROPERTIES OF INSULATORS

Investigators: J. J. Markham

Scope of Work:

The purpose of this program is to understand the magnetic and optical properties of the F-center in a quantitative manner. The F-center in alkali halides is one of the most thoroughly studied point imperfections. The paramagnetic resonance absorption signal is broadened by hyperfine interactions between the electron trapped at an imperfection (negative-ion vacancy) and the surrounding nuclei. At low temperatures, one may saturate a portion of the absorption without affecting the other portions, provided one uses dilutely colored crystals. Measurements of the spin lattice relaxation and the coupling between the spins are possible. These studies are now being made on additively colored KCl and RbCl.

During the work on this contract, it has been discovered that certain corrections are required to Portis' theory of inhomogeneous broadening. Attempts have been made to show the nature of these corrections. Carefully taken data show these modifications are necessary. The analysis also indicates that the magnetic signal obtained from bleached F-centers can be ascribed to one paramagnetic imperfection which does not seem to be the F-center. Theoretical studies of the vibrations about point imperfections show that the lattice modes are modified at points where the crystal is imperfect. These modifications are of great importance for phenomena pertaining to short range interactions between electrons and ions. A study of these effects has been made.

Contractor: Armour Research Foundation, Chicago, Illinois

Contract Number: AT(11-1)-578, Proj. No. 19

Present Contract Term: March 15, 1962 through March 14, 1963

Cost to AEC: $27,170

Contract Title: ALLOYING CHARACTERISTICS OF THE RARE EARTH ELEMENTS WITH THE TRANSITION ELEMENTS

Investigators: Rodney P. Elliott

Scope of Work:

The alloying characteristics of the rare earth elements with the transition metals undergo a radical change in nature as the atomic number of the transition series increases--transition elements in Groups IV a, V a, and VI a are immiscible with the rare earths, while elements of Groups VII a, and VIII a, VIII b, and VIII c form many compounds. A reasonable explanation for this behavior is a valency or electronegativity effect. Those binary systems forming compounds form "Laves phases", which can exist in one of three related crystal sturctures. The specific Laves type crystal structure can be related to the average free electron concentration. This phenomenon has been used previously to calculate electronic valency of other systems. From a thorough compilation of the known Laves-type phases occurring between rare earth elements and transition metals, the crystal structure trend supports the hypothesis that the valency effect is indeed operative, however, further substantiation of these trends are dictated. In the present program, uninvestigated rare earth-transition metal binary systems are being surveyed to establish the existence or non-existence of the Laves type phase and to classify the crystal sturcture of observed Laves phases. Alloying between Laves phases of unlike crystal structure will then be made to establish solubility limits from which valencies will be calculated.

Contractor: Atomics International, A Division of North American Aviation, Inc., Canoga Park, California

Contract Number: AT(11-1)-Gen-8

Present Contract Term: July 1, 1962 through June 30, 1963 (Fiscal year 1963)

Cost to AEC:

Contract Title: SOLID STATE PHYSICS AND DEFECT PROPERTIES

Investigators: A. Sosin, T. G. Berlincourt and staff

Scope of Work: A. Electronic Structure of Metals and Alloys
T. G. Berlincourt, J. A. Cape, R. R. Hake, D. H. Leslie, A. C. Thorsen, and W. J. Tomasch

This project is concerned with studies of properties which can be directly related to the electronic character of metals, emphasis being placed upon transition metals and their alloys. de Haas-van Alphen effect studies of single crystals of pure metals and intermetallic compounds are used to deduce the detailed shape of the Fermi surface, and gross features of the electronic structure are revealed by conventional magnetic susceptibility and low temperature specific heat studies. The latter measurements yield values for the total energy density of electronic states at the Fermi surface and are carried out on polycrystalline disordered alloys as a function of alloying concentration. Measurements of electron tunneling, electrical resistivity, magnetoresistivity, and Hall effect are also used to characterize the electronic structure. Considerable emphasis has recently been devoted to attempts to understand the unusual properties of alloy superconductors in very high magnetic fields.

Recent progress on this project has been marked by (1) the first observations of the de Haas-van Alphen effect in Rb, Nb, Ta, Zr, Th, and the metallic intermetallic compound InBi; (2) the demonstration that modified negative surface energy theory can account quantitatively for the upper critical fields of transition metal alloy superconductors; (3) clarification of the role of anisotropic defect structure in the superconducting properties of alloy superconductors; (4) the production of magnetic fields up to 60 kilogauss with Nb-Zr alloy superconducting solenoids; (5) the demonstration that Ti-Nb alloys may be suitable for 100 kilogauss superconducting magnets; (6) the observation that localized magnetic states exist in dilute Ti-Mn alloys despite the fact that addition of dilute quantities of Mn to Ti raises the superconducting transition temperature markedly; and (7) the observation of unusual electron tunneling transport between antiferromagnetic and superconducting materials.

B. Defect-Controlled Processes in Metals and Alloys

A. Sosin, C. J. Meechan, D. Kramer

It is the purpose of this program to obtain information about the factors governing the nature of the diffusive motion of atoms, leading to such phenomena as segregation and phase reversion. Emphasis is placed on vacancy-controlled processes in metals.

The formation of Guinier-Preston zones in Al-Zn alloys ranging in composition from 1.7 to 5.3 atomic percent Zn has been investigated by electrical resistivity measurements.

A maximum was found to occur in the resistivity during isothermal aging at low temperatures (-60 to 0°C) subsequent to a rapid quench from 300 or 450°C. However, the time at which the maximum occurs did not yield a straight line on an Arhennius plot and no activation energy could be obtained.

A series of quenching measurements were made in Al-0.1 at .% Zn. The excess resistivity due to quenching is found to obey an Arhennius equation with an activation energy between 0.695 and 0.72 ev. The annealing spectrum is qualitatively similar to that reported by Panseri and Frederighi; however, the recovery stages appear to be shifted to lower temperatures. A direct comparison between alloy samples and pure aluminum samples is being attempted to verify this effect.

C. Radiation Damage in Crystalline Solids

A. Sosin, F. H. Eisen, D. W. Keefer, and W. Bauer

The energy dependence of the damage rate and the recovery of each substage in Stage I in pure copper as a function of electron energy has been studied. The damage rate has been fitted to a theoretical calculation of displacement cross-section which attempts to evaluate the probability that an atom is displaced, considering only the (110) directions in detail. Techniques have been developed to permit the irradiation of single crystal foils of copper less than 0.0005 inches thick. Irradiation of such samples which are aligned so that the electron beam impinges along a (100) or (110) direction should permit a determination of the directional dependence of displacements in copper.

Changes in elastic modulus and internal friction resulting from irradiation which are ascribed to pinning of dislocations by irradiation-produced defects, have been found to anneal out at temperatures over 200°C. Activation energies for this annealing are quite high, indicating that the pinning defects are not simple in nature.

Studies of electron radiation damage in InSb have been extended to p-type material where the recovery is more complex than in n-type InSb. Some of the changes in recovery have been interpreted as due to the effects on the recovery of changes in the charge state of the defects. The polarity in the (111)

direction of InSb suggests that it may be possible to observe assymetries in damage between opposite sides of samples with (111) faces. Studies of this should permit the identification of the atoms displaced in producing defects by electron irradiation of InSb.

Recent Publications:

A. C. Thorsen, T. G. Berlincourt, "deHaas-van Alphen Effect in Rhenium, Niobium, and Tantalum," Phys. Rev. Ltrs. 7, (1961) p. 244.

R. R. Hake, T. G. Berlincourt, and D. H. Leslie, "High Field Superconductivity in Some bcc Ti-Mo and NB-Zr Alloys," IBM J. Research Develop 6, (1962) p. 119.

R. R. Hake, D. H. Leslie and T. G. Berlincourt, "Low Temperature Resistivity Minima and Negative Magnetoresistivities in Some Dilute Superconducting Ti Alloys," Phys. Rev. (in press).

J. F. Hon, "A Nuclear Magnetic Resonance Study of the Diffusion of Hydrogen in Zirconium Hydride," J. Chem. Phys. (in press).

A. C. Thorsen and T. G. Berlincourt, "deHaas-van Alphen Effect in InBi," Nature 192, (1961) p. 959.

R. R. Hake, T. G. Berlincourt, and D. H. Leslie, "A 59 Kilogauss Niobium-Zirconium Superconducting Solenoid," High Magnetic Fields, (M.I.T. Press, Cambridge, and John Wiley & Sons, Inc., New York, 1962), pp 341-343.

R. R. Hake, T. G. Berlincourt, and D. H. Leslie, "Characteristics of some High Field Superconductors," Bull. Am. Phys. Soc. 6, (1961) p. 425.

T. G. Berlincourt, R. R. Hake, and A. C. Thorsen, "Pulsed Magnetic Field Studies of the Negative Magnetoresistivities of Dilute Ti-Mn and Cu-Mn Alloys at Low Temperatures," Bull. Am. Phys. Soc. 6, (1961) p. 502.

A. C. Thorsen and T. G. Berlincourt, "deHaas-van Alphen Effect in Rubidium," Bull. Am. Phys. Soc. 6, (1961) p. 511.

R. R. Hake, "Superconductivity in Transition Metal Alloys," Bull. Am. Phys. Soc. 6, (1961) p. 505.

A. C. Thorsen, "deHaas-van Alphen Effect in Alkali and Transition Metals," Bull. Am. Phys. Soc. 7, (1962) p. 222.

T. G. Berlincourt, R. R. Hake, and A. C. Thorsen, "Pulsed Magnetic Field Studies of the Negative Magnetoresistivities of Dilute Ti-Mn and Cu-Mn Alloys at Low Temperatures," Phys. Rev. (in press).

R. R. Hake, T. G. Berlincourt, and D. H. Leslie, "High-Field Superconducting Characteristics of Some Ductile Transition Metal Alloys," Proceedings of the 1962 AIME Symposium on Superconducting Materials, (Interscience, New York), in press.

R. R. Hake and D. H. Leslie, "High-Field Superconducting Properties of Ti-Mo Alloys," Physics. Rev. (submitted).

T. G. Berlincourt and R. R. Hake, "Pulsed-Magnetic-Field Studies of Superconducting Transition Metal Alloys at High and Low Current Densities," Bull. Am. Phys. Soc. 7, (1962) p 408

G. W. Lehman, "Temperature Distribution in a Hollow Cylindrical Cup with a Stem," J. of Appl. Phys., 33, (1962) p. 629.

C. J. Meechan and G. W. Lehman, "Diffusion of Au and Cu in a Temperature Gradient, " J. of Appl. Phys, 33, (1962) p 634.

A. Grenall, "Electron Microscope Observations of Fast Neutron Damage in Gold Films," J. of Nuc. Mat'l. 4, (1961) p. 330.

J. A. Brinkman, A. Sosin, and A. Grenall, "An Interpretation of Electron Microscope Observations in Neutron-Irradiated Copper and Gold." J. Nuc. Mat'l. 4, (1961) p. 332.

A. Sosin, "The Energy Dependence of Electron Damage in Copper," Phys. Rev., June 1962.

A. Sosin and H. H. Neely, "A Cryostat for Irradiating at 4.2°K," Rev. Sci. Inst. 32, (1961) p. 922.

L. H. Rachal, "A Fast Response, Low Inertia Vacuum Furnace," Rev. Sci. Inst. 32, (1961), p. 940.

F. H. Eisen, "Recovery of Electron Radiation Damage in n-type InSb," Phys. Rev. 123, (1961) p. 736

A. Sosin and H. H. Neely, "The Influence of Foreign Solute Atoms on Stage I Recovery in Electron-Irradiated Copper," Submitted to Phys. Rev.

A. Sosin, "Dislocation Pinning in Copper at 4.2°K and in Stage I," submitted to J. Appl. Phys.

Contractor:	Battelle Memorial Institute, Columbus, Ohio
Contract Number:	W-7405-ENG-92
Present Contract Term:	July 1, 1962 through June 30, 1963 (Fiscal year 1963)
Cost to AEC:	$26,335
Contract Title:	THE CHARGE OF INTERSTITIAL IONS IN GROUPS IV-A AND V-A TRANSITION METALS
Investigators:	Peter S. Rudman

Scope of Work:

One of the important roles of interstitial solutes in metallic solid solution may be as donors or acceptors of electrons. This role has been studied to some extent mainly be means of electron band and transport properties (e.g., magnetic susceptibility, electrical resistivity, etc.). While the present study will include this type of measurement, the major emphasis will be on the complementary determination of the charge on the resulting interstitial ion by means of interstitial migration in a d-c electric field. This technique is not new to this problem, but heretofore the few studies that have been made have been of dubious value. This failure can be attributed to two causes: (1) experimental inaccuracy and (2) inadequate theory. It appears that the necessary experimental and analytical chemical techniques have now been sufficiently refined to justify d-c migration studies. Also, a recent theoretical "break-through" by Huntington now apparently allows a "true interstitial charge" to be derived from the experimentally determined "apparent interstitial charge". Thus the state of the art and theory indicate that meaningful and quantitative interstitial d-c migration studies may now be possible.

The present experiments will be initiated on some as yet unspecified interstitial Group IV-A or Group V-A binary system that appears to be the most tractable by virtue of experimental convenience and the availability of good interstitial diffusion data.

Contractor: Bausch & Lomb Incorporated, Rochester, New York

Contract Number: AT(30-1)-1312

Present Contract Term: January 1, 1962 through December 31, 1962

Cost to AEC: $20,000

Contract Title: IRRADIATION DAMAGE TO GLASS

Investigators: N. J. Kreidl

Scope of Work:

This research is concerned with the effects of high energy radiation on some of the optical, electrical, and mechanical properties of glasses. Co^{60} gamma rays and 1.5 MeV electrons were used. The work at present falls mainly into two categories: effects of radiation on fused silica compressed under high pressure, and effects of radiation on electrical conductivity of various glasses. Work on high pressure effects is being pursued with the tetrahedral device described in the November 1961 report. Pressures up to 100 kilobars can be obtained. The device has been calibrated for pressure; temperature calibration will be completed soon. High temperatures and pressures have been applied to small cylinders of fused silica; the most useful range of pressure and temperature for subsequent radiation studies will be determined. The effects of high pressure on glass melted under oxidizing and reducing conditions is under study. Absorption and density differ according to the atmosphere used. In the conductivity studies, measurements are being carried out on fused silica, lead silicate glass, phosphate glass, and Pyrex. Cycles of measurements on charging and discharging currents have been made which show several distinct relaxation times. These are being correlated with structure when possible.

Contractor: Brown University, Providence, Rhode Island

Contract Number: AT(30-1)-2024

Present Contract Term: May 1, 1962 through April 30, 1963

Cost to AEC: $49,916

Contract Title: RADIATION DAMAGE STUDIES IN SOLIDS USING MAGNETIC RESONANCE TECHNIQUES

Investigators: Philip J. Bray

Scope of Work:

The major effort is to obtain a closer unification of nuclear magnetic resonance (NMR) techniques, electron-spin paramagnetic resonance (ESR) techniques, and auxiliary techniques such as optical investigations used to study more thoroughly the mechanisms of defect formation in alkali-halide single crystals, semiconductor materials, and several non-cubic materials. Particular attention is given to the preparation of the alkali halide crystals and the subsequent handling of the materials before and after irradiation. The effects on the defect structure in these materials after irradiation will be examined as a function of compressing, annealing, cooling, and the condition of the crystal surfaces.

The studies of conduction electrons in metal specks formed in irradiated alkali halides will be extended in an attempt to obtain more information as to the size, position and the detailed nature of these metallic specks. The study of ESR resonances due to atomic hydrogen and tritium trapped in irradiated alkali halides will be continued to obtain information concerning the position of these atoms in the crystals and the interactions of these atoms with the ions of the normal lattice. The ESR studies of defects and color centers produced in irradiated alkali borate and alumino silicate glasses will be continued and extended to other glass systems. The interpretations of the ESR spectra from the irradiated alkali borate and alumino silicate glasses will be checked further and extended to other glass systems where applicable.

Recent Publications:

Sook Lee and P. J. Bray, "Electron-Spin Paramagnetic Resonance of Irradiated Alumino-Silicate Glasses," J. of Soc. of Glass Tech., Section B. Physics and Chemistry of Glass, April 1962.

R. Kaplan and P. J. Bray, "Exchange Narrowing of the F-center Electron Spin Resonance in Neutron-Irradiated LiF," Submitted to Phys. Rev. December, 1961.

C. D. Knutson and P. J. Bray, "Nuclear Magnetic Resonance Studies of Neutron-Irradiated LiF," Submitted to the J. of Phys. and Chem. of Solids.

Sook Lee and P. J. Bray, "Electron Paramagnetic Resonance of Irradiated Borosilicate Glasses," BAPS II 6, (1961) p. 246.

Charles D. Knutson and P. J. Bray, "NMR of Neutron-Irradiated LiF," BAPS II 6, (1961) p. 19.

Charles D. Knutson and P. J. Bray, "Radiation Damage in Crystalline Fluorides," BAPS II 6, (1961) p. 113.

J. A. Dweck and P. J. Bray, "Paramagnetic Resonance Investigations of Atomic Hydrogen and Tritium in Neutron-Irradiated Crystalline Fluorides," BAPS II 6, (1961) p. 113.

J. A. Dweck, H. O. Hooper, and P. J. Bray, "Electron Spin Resonance Investigations of Atomic Hydrogen and Tritium in Neutron-Irradiated Crystalline Fluorides," BAPS II 7, (1962) p. 51.

A. C. Greene, H. O. Hooper, and P. J. Bray, "NMR of Neutron-Irrdiated KBr," BAPS II 7, (1962) p. 51.

Contractor: Brown University, Providence, Rhode Island

Contract Number: AT(30-1)-2394

Present Contract Term: June 1, 1962 through May 31, 1963

Cost to AEC: $13,290

Contract Title: ANALYSIS OF STRUCTURES OF TWO-PHASE ALLOYS

Investigators: Joseph Gurland

Scope of Work:

The purpose of this work is to permit a rationalization of the observed variation of strength with composition and grain size, on the basis of theoretical considerations of fracture initiation at inclusions, plastic constraint of the ductile matrix in contact with rigid particles, and fracture propagation through the brittle phase as a function of structural continuity.

The principal effort is devoted to a study of the fracture strength of two-phase alloys. Experimentally, the work will be done on suitable brittle-ductile composites such as tungsten carbide - cobalt and aluminum - silicon two-phase aggregates. The variable parameters are the composition and the grain size of the brittle phase and the measured data will consist of the static fracture strength in bending and tension, the elongation at rupture, the impact strength, the hardness and the yield strength. It is intended to carry out the measurement of mechanical properties over as wide a range of composition as possible, preferably over the entire range of the binary mixtures. The particular binary systems were selected because their fracture behavior has already been studied from a structural point of view and it is known that these alloys fail by fracture initiation within the brittle constituents (i.e. WC and Si).

Contractor: California Institute of Technology, Pasadena, California

Contract Number: AT(04-3)-221

Present Contract Term: June 1, 1962 through May 31, 1963

Cost to AEC: $140,000

Contract Title: FUNDAMENTAL STUDIES OF MATERIALS PERTAINING TO NUCLEAR ENGINEERING

Investigators: Pol Duwez

Scope of Work:

The work on the structure of alloys very rapidly cooled from the melt has progressed in three directions: 1) extension of limits of solid solubility, 2) new intermediate phases not obtained under equilibrium conditions, 3) Amorphous alloys. The solubility limits of tin, germanium and silicon in nickel can be substantially increased by fast cooling. Similar results have been obtained in copper-cobalt and gold-cobalt alloys. A number of new intermediate phases have been discovered. A most unusual crystal structure (simple cubic with one atom per unit cell) has been found in binary alloys of tellurium with silver and gold. This new phase appears to be a semi-conductor. Amorphous phases have been found in binary alloys of tellurium with germanium. These alloys are stable at room temperature. Electron microscopy studies revealed that crystallization takes place by dendritic growth within the amorphous matrix. The physical properties of these new alloys are now being studied, including electrical, magnetic and superconducting properties.

Recent Publications:

W. Klement, Jr., "Lattice Parameters of the Metastable Close-Packed Hexagonal Structures in Silver-Germanium Alloys," J. Institute of Metals, 90, (1961) pp. 27-30.

H. L. Luo and W. Klement, Jr., "Metastable Simple Cubic Structures in Gold-Tellurium and Silver-Tellurium Alloys," J. of Chemical Phys., April, 1962.

K. Krishna Rao, "Electrical Resistivity Recovery in Cold-Worked Sixty Percent Silver-Forty Percent Palladium Alloy," Accepted for publication in Acta. Met.

R. H. Willens, "A New Method for Preparing Specimens for Transmission Electron Microscopy," Proceedings of the Fifth International Conf. in Electron Microscopy, Philadelphia, 1962, Vol. I, pp. EE-6.

Contractor:	California Institute of Technology, Pasadena, California
Contract Number:	AT(04-3)-473
Present Contract Term:	November 1, 1962 through October 31, 1963
Cost to AEC:	$20,000
Contract Title:	A STUDY OF DISLOCATION MOBILITY AND DENSITY IN METALLIC CRYSTALS
Investigators:	D. S. Wood and T. Vreeland, Jr.

Scope of Work:

While a considerable amount of knowledge about dislocations in crystals has evolved during the past 30 years, very little is known about the factors which limit dislocation mobility. It is therefore impossible to predict the strain and strain rate resulting from the application of a stress to a crystal, even when the dislocation density and arrangement are known.

Experiments are under way which will permit determination of dislocation density and mobility in crystals wherein such variables as the initial dislocation density and arrangement, temperature, concentration of impurities, vacancies, and interstitials are carefully controlled. These experiments will be guided by theoretical studies whenever possible in an attempt to develop quantitative theories of the effects of the above mentioned variables on dislocation mobility and density.

Dislocation densities will be determined by etch pit techniques, and, where practical, by electron microscopy of thinned crystals. Dislocation mobility will be determined by measurement of dislocation displacements produced by stress pulses of controlled amplitude and duration. Systems capable of producing single stress pulses as short as 5 micro sec in duration are being assembled.

Contractor: California, University of, Berkeley, California

Contract Number: AT(11-1)-34, Proj. No. 47

Present Contract Term: August 1, 1962 through July 31, 1963

Cost to AEC: $45,000

Contract Title: MICROWAVE FARADAY ROTATION AND OTHER STUDIES

Investigators: Alan M. Portis

Scope of Work:

The work being done on this project is largely concerned with the magnetic properties of insulating and metallic solids. The primary techniques used are nuclear and electron resonance.

An extensive program is in progress involving single crystals of chemical composition $XMnF_3$ where X is an alkali atom. These crystals become ordered antiferromagnetically below some temperature between 50 and 90°K. There are three principal reasons for studying this class of crystals: (1) their crystal structure is simple so that an understanding of exchange interaction is feasible; (2) the highly symmetrical crystal structure together with divalent manganese make for low magnetic anisotropy, simplifying the observation of antiferromagnetic resonance; (3) the low anisotropy together with the large magnetic moment of Mn^{55} produces strong nuclear-electronic interactions making possible the observation of nuclear-antiferromagnetic double resonance. In addition to extending our initial studies of $KMnF_3$ to the other crystals in this group we are also investigating the spectrum of nuclear excitations in these crystals and the possibility of the propagation of such excitations.

In addition investigations of the following metallic problems are in progress: (1) nuclear magnetic resonance in ferromagnetic alloys, (2) transport properties of the ordered heavy rare earth metals, and (3) microwave Faraday rotation in superconducting and ferromagnetic metals.

Recent Publications:

Dale T. Teaney, M. P. Klein, and A. M. Portis, "A Microwave Superheterodyne Induction Spectrometer, Rev. Sci. Instr. 32, (1961) p. 721.

A. J. Heeger, A. M. Portis, Olof Beckman, "Magnetic Properties of $KMnF_3$. II. Weak Ferromagnetism," Phys. Rev. 123, 1961, p. 1652.

A. J. Heeger, A. M. Portis, Dale T. Teaney, and Gerald Witt, "Double Resonance and Nuclear Cooling in an Antiferromagnetic," Phys. Rev. Letters 7, 1961, p. 307.

A. J. Heeger, A. M. Portis, and Gerald Witt, "Double Nuclear Antiferromagnetic Resonance," Presented at the International Conference on Magnetic and Electric Resonance and Relaxation, Eindhoven, July, 1962.

A. M. Portis and J. Kanamori, "Interpretation of NMR Spectra in Ferromagnetic Alloys," J. Phys. Soc. Japan 17, 1962, p. 587.

Allan Zalkin, Kenneth Lee, and David H. Templeton, "The Crystal Structure of $CsMnF_3$. Submitted to the J. of Physics and Chemistry of Solids.

Contractor: California, University of, Berkeley, California

Contract Number: AT(11-1)-34, Proj. No. 76

Present Contract Term: January 1, 1963 through December 31, 1963

Cost to AEC: $22,000

Contract Title: PHONON RESEARCH IN SOLIDS (PRS)

Investigators: Klaus Dransfeld

Scope of Work:

This project was initiated to provide support for research on phonons in solids and liquid helium. During the past year progress has been made on the study of spin-phonon interaction in ferrites by completion of construction of equipment and the developing of bonding techniques for attaching samples to piezoelectric quartz rods. Measurememts have begun on absorption of longitudinal acoustic waves in Yig as a function of temperature and magnetic field.

A change in the velocity of sound in indium when going from the normal to the superconducting state has been sought, the change being anticipated because of a reported large change in specific heat. More recent data has not confirmed the specific heat changes and thus the velocity measurements have been postponed. In stead, work is under way on the microwave ultrasonic absorption of superconductors. Equipment has been perfected, vandium crystals obtained, oriented, cut and polished. Measurements are about to be made.

Other studies include infrared absorption in LiF as a function of temperature down to 20°K. A T^2 law was found to describe the results while first indications in NaCl show linear dependence. Theoretical work on acoustic absorption and superfluid helium has been brought to a point where a paper has been published in the Physical Review.*

Recent Publications:

K. Dransfeld, "Ultrasonic Absorption in Liquid Helium at Temperatures below o.6°K," Phys. Rev. 127, (1962) p. 17.

K. Dransfeld, "Dielectric Relaxation of Water Adsorbed on γ-Alumina," Journal Chem. Phys. 36, (1962) p. 1574.

Contractor: California, University of, Riverside, California

Contract Number: AT(11-1)-34, Proj. No. 77

Present Contract Term: May 1, 1962 through July 31, 1963

Cost to AEC: $54,410

Contract Title: PRESSURE INDUCED METALLIC CONDUCTIVITY IN TRANSITION METAL OXIDES AND RELATED COMPOUNDS

Investigators: A. W. Lawson

Scope of Work:

This contract is devoted primarily to high pressure studies of the electrical and magnetic properties of transition metals and their compounds. The previous work on high pressure X-ray studies has been extended into the 100 kbar range and efforts are being made to study the phase transitions in Cs with hopes of coupling such studies with a search for superconductivity or ferromagnetism in the high pressure modifications. In addition, the electrical conductivity of such compounds as MnS are being studied as a function of pressure to study the trend towards metallic conductivity in these systems. The cubic ferromagnetic EuS is currently under study to determine the shift in the 20°K Curie temperature with pressure. Instrumentation has been developed for studies of ferromagnetic resonance under pressure at 1cm and will be applied to a number of systems accessible at room temperature in fields up to 15kg and pressures up to 10kb. These experiments are designed to elucidate the role of overlap forces in ferromagnetic materials.

Contractor:	California, University of, Los Angeles, California
Contract Number:	AT(11-1)-34, Proj. No. 103
Present Contract Term:	June 1, 1963 through May 31, 1964
Cost to AEC:	$36,244
Contract Title:	SPECTROSCOPIC STUDY OF LATTICE VIBRATIONS IN CRYSTALLINE SOLIDS
Investigators:	R. A. Satten

Scope of Work:

The vibrational spectra of solids is being studied by three spectroscopic approaches: far infrared, Raman, and vibronic.

The far infrared spectrum from 300 cm^{-2} down to at least 50 cm^{-1} is being studied to obtain the fundamental lattice vibrations of those crystals whose lattice vibrations, have already been studied indirectly coupled to electronic transitions. Initial work is on Cs_2UCl_2, $[N(CH_3)_4]_2UCl_6$ and $[N(C_2H_5)_4]_2UCl_6$. These measurements will be supplemented by measurement of the Raman spectra. Studies of the vibronic transitions have been completed. Also a program of theoretical calculation of the lattice vibrations of crystals that have been studied experimentally, is under way.

Past research at UCLA on the electron-phonon transitions associated with the presence of actinide ions in crystals has shown that this is a useful technique for studying the lattice vibrations of a crystal over the entire range of the spectrum. This work is being extended to learn the influence of the concentration of actinide ion, using U^{+4} in Cs_2ZrCl_6.

Other problems involving actinide ions in crystal lattices are also being pursued.

Contractor: Carnegie Institute of Technology, Pittsburgh, Pennsylvania

Contract Number: AT(30-1)-2314

Present Contract Term: January 1, 1963 through December 31, 1963

Cost to AEC: $29,960

Contract Title: SURFACE DIFFUSION ON METALS

Investigators: Paul G. Shewmon

Scope of Work:

Twist type grain boundaries in silver are being made by sintering two single crystals together. Preliminary results indicate that the diffusion coefficients in these twist boundaries (D_b) is roughly a factor of 5 slower than a tilt type boundary of the same misorientation. Measurements of D_b will be made over a range of angles in twist boundaries containing the (100) plane as well as in a few boundaries containing (110) or (111) planes. The temperature dependence of D_s will be checked for a few boundaries.

The variation of the surface diffusion coefficient (D_s) with direction in a surface and orientation of the surface is being studied on copper. The values of D_s are obtained from the kinetics of smoothing of a scratch in an otherwise flat surface. Where possible, these will be compared with the values obtained from the kinetics of grain boundary grooving. During the latter part of the year we shall attempt to measure D_s by a tracer technique and compare the tracer results with those obtained by the grooving method.

Recent Publications:

P. G. Shewmon and J. Y. Choi, "Anisotropy of the Surface Diffusion Coefficient for Copper," Submitted to Trans. AIME.

P. G. Shewmon, "Surface Diffusion from a Point Source," Submitted to Jnl. Appl. Physics.

J. Choi and P. G. Shewmon, "Effect of Orientation on the Surface Self-Diffusion of Copper," Submitted to Trans. AIME.

H. M. Robertson and P. G. Shewmon, "Variation of Surface Tension with Surface Orientation in Copper," Submitted to Trans. AIME.

Contractor: Carnegie Institute of Technology, Pittsburgh, Pennsylvania

Contract Number: AT(30-1)-2360

Present Contract Term: March 15, 1962 through March 14, 1963

Cost to AEC: $24,467

Contract Title: THERMAL CONDUCTIVITY OF INORGANIC MELTS

Investigators: W. O. Philbrook

Scope of Work:

Preliminary values have been obtained for the thermal conductivity of molten silver sulfide near the stoichiometric composition of Ag_2S at 830 - 950°C and for molten silver containing 7.5 a/o sulfur at 1020°C, using a steady-state apparatus of cylindrical geometry constructed of graphite. Minor revisions in the apparatus are being made to eliminate thermoelectric interference.

The order of magnitude of the thermal conductivity of Ag_2S is consistent with the electrical properties of the melt and a model based on phonon and diffusional transport plus an electronic contribution calculated from the classical Lorenz No. for non-degenerate electron gas. The role of paired electron-hole conduction is probably small if the preliminary data are confirmed. The high thermal conductivity of the silver-rich melt is consistent with its electrical behavior as a metallic conductor.

Future plans include verification of the present data to demonstrate the absence of significant interference from convection, radiation or thermoelectric effects and extension of measurements to the molten sulfides of Ni and Tl, with interpretation in terms of structural models suggested by electrical properties of these melts.

Contractor: Carnegie Institute of Technology, Pittsburgh, Pennsylvania

Contract Number: AT(30-1)-3001

Present Contract Term: May 1, 1962 through April 30, 1963

Cost to AEC: $28,458

Contract Title: A STUDY OF THE INTERACTION BETWEEN POINT DEFECTS AND DISLOCATIONS THROUGH DISLOCATION DAMPING EXPERIMENTS

Investigators: Charles L. Bauer

Scope of Work:

A number of experiments are proposed utilizing elastic modulus and internal friction measurements to investigate some of the structure-sensitive properties of crystals. Initially, a study of thermally activated dislocation pinning in the alkali halides will be conducted to yield information concerning the mechanical damping. A test of the revised Granato-Lücke theory will also be conducted by observing the strain amplitude dependence of the internal friction at low temperatures as traces of known impurities are added to metallic single crystals. Another proposed project is to investigate the "strength" of the interaction of impurities with dislocations at high temperatures by using the dislocation damping technique to measure the concentration of impurities actually located on the dislocation lines. The final project, which should demonstrate the electronic nature of dislocation pinning in the alkali halides, will utilize internal friction and elastic modulus measurement to observe dislocation damping as a function of the energy of incident ultraviolet irradiation.

Contractor: Carnegie Institute of Technology, Pittsburgh, Pennsylvania

Contract Number: AT(30-1)-3033

Present Contract Term: April 1, 1962 through March 31, 1963

Cost to AEC: $36,770

Contract Title: RADIATION EFFECTS IN SOLIDS

Investigators: D. A. Wiegand

Scope of Work:

Radiation effects in ionic crystalline solids are being studied in an effort to obtain answers to the following two questions: a) What are the types of defects that can be introduced by ionizing irradiation; and b) By what mechanism or mechanisms are these defects generated? An answer to one of these questions will undoubtedly provide at least a partial answer to the other question. In particular, attempts will be made to establish the nature of defects complimentary to the negative ion vacancy. Since it appears that possible complimentary defects other than the H center are not detectable by paramagnetic resonance, techniques such as x-ray diffraction, and optical absorption will be used. The macroscopic expansion will also be investigated. Studies of defect symmetry will be made by the use of polarized light techniques.

Kinetic studies of the rate of defect production as a function of such parameters as temperature, sample perfection and intensity will be made. It is expected that definite limitations can be placed upon the possible mechanisms of defect production by information obtained in this manner.

The interaction of dislocations with the products of ionizing radiation will also be investigated.

Recent Publications:

R. E. Howard, S. Vosko, and R. Smoluchowski, "Mechanism for Production of Interstitials in KCl by X-Rays at Low Temperatures," Phys. Rev. 122, (1961), p. 1406.

R. Smoluchowski and D. A. Wiegand, "The Formation of Interstitials and Vacancies in Alkali Halides," Discussions of the Faraday Society, #31, (1961) p. 151.

P. V. Mitchell, D. A. Wiegand, and R. Smoluchowski, "Formation of F Centers in KCl by X-Rays," Phys. Rev. 121, (1961) p. 484.

M. F. Merriam, D. A. Wiegand, and R. Smoluchowski, "Enhanced Thermal Expansion in X-Rayed Rocksalt," Phys. Rev. 125, (1962), p. 52.

M. F. Merriam, R. Smoluchowski, and D. A. Wiegand, "High-Temperature Thermal Expansion of Rocksalt," Phys. Rev. 125, (1962), p. 65.

D. A. Weigand and R. Smoluchowski, "X-Ray Induced Defects in LiF Crystals Plastically Deformed at Low Temperatures," Bull. Amer. Phys. Soc. II 6, (1961), p. 113.

Contractor: Case Institute of Technology, Cleveland, Ohio

Contract Number: AT(11-1)-588

Present Contract Term: November 1, 1962 through October 31, 1963

Cost to AEC: $23,500

Contract Title: KINETICS OF PHASE TRANSFORMATIONS IN ZIRCONIUM-NIOBIUM ALLOYS

Investigators: R. F. Hehemann

Scope of Work:

The omega transformation can occur during quenching without compostion change or isothermally where decomposition is accompanied by enrichment of the parent phase in solute. The athermal transformation is associated with an increase in electrical resistivity and is thermally reversible with virtually no hysteresis. This gives rise to a negative temperature coefficient of resistivity at temperatues below room temperature in an alloy having 17% niobium.

An analysis of diffuse diffraction effects associated with omega formed during quenching reveals that the transformation product exists initially as planar zones (on (112) planes) analogous to the zones observed in many age hardening systems. However, the β "average" lattice of the zones in these alloys approximates that of the precipitate (omega) rather than that of the matrix as is characteristic of the majority of the age hardening systems. While substitutional disorder is of primary importance in most age hardening systems, displacement disorder plays a dominant role in the zonal structure of omega. It is this phenomenon that gives rise to the apparent "rumpled" central plane that has been employed to describe the structure resulting from the early stages of this transformation.

Vacancies play an important role in the development of the zones and their conversion to the final equilibrium structure. A model for the transformation based on the relaxation which occurs around single vacancies and vacancy aggregates is under development.

Contractor: Case Institute of Technology, Cleveland, Ohio

Contract Number: AT(11-1)-623

Present Contract Term: February 1, 1962 through January 1, 1963

Cost to AEC: $74,000

Contract Title: SOLID STATE PHYSICS

Investigators: C. S. Smith

Scope of Work:

The work in progress and proposed is directed to the experimental study of thin film physics and the cohesive properties of solids and to the theoretical study of the band structure, transport properties, statistical mechanics and lattice dynamics of solids.

The work in thin film physics will center about the new ultra high vacuum system and deals with the magnetic, electrical, mechanical and crystallographic properties of metal films prepared under the best conditions possible today.

The specific cohesive properties under study are the low temperature thermal expansion and the related pressure variation of the elastic constants. The work will deal primarily with the alkali halides and is directed toward relating these properties to the microscopic interactions in the crystal.

Three theoretical studies concerning lattice anharmonicity, thermal expansion and lattice dynamics will provide a general base for the interpretation of the experimental studies of the preceding paragraph. Other theoretical studies in statistical mechanics, transport phenomena and band structure in solids reflect the special interests of our theorists.

Recent Publications:

J. R. Reitz, R. N. Seitz, and R. W. Genberg, "Closed-Shell Ion-Ion Interactions in Calcium Fluoride," J. Phys. Chem. Solids 19, (1961), p. 73.

J. R. Reitz, "Peltier Coefficient at High Current Levels," J. Appl. Phys. 32, (1961), p. 1623

Van E. Wood and J. R. Reitz, "Electronic Band Structure of Cesium Gold," Accepted for publication in J. Phys. Chem. Solids.

A. S. Joseph, W. L. Gordon, J. R. Reitz, and T. G. Eck, "Evidence for Spin-Orbit Splitting in the Band Structure of Zinc and Cadmium," Submitted to Phys. Rev. Letters.

M. J. Klein, "Pressure Fluctuations," Physica 26, (1960), pp. 1073-1079.

A. Yelon, J. R. Asik, and R. W. Hoffman, "Fiber Texture and Magnetic Anisotropy in Evaporated Iron Films," Submitted to Journal Appl. Phys.

S. Eros and Charles S. Smith, "Low Temperature Elastic Constants of Magnesium Alloys," Acta Metallurgica, 9, (1961), p. 14.

J. Trivisonno and Charles S. Smith, "Elastic Constants of Li-Mg Alloys, Accepted by Acta Metallurgica.

Contractor: Catholic University of America, Washington, D.C.

Contract Number: AT(40-1)-2861

Present Contract Term: June 1, 1962 through August 31, 1963

Cost to AEC: $64,720

Contract Title: ULTRASONIC STUDIES OF ALKALI METALS

Investigators: Paul H. E. Meijer

Scope of Work:

The electronic structure of solids are being studied using ultrasonic attenuation techniques. One of the main areas of study is the Fermi surface of the alkali metals. For this purpose, techniques of production of pure, oriented single crystals of potassium are being worked out. One crystal about one centimeter on a side has been produced. Using crystals such as this, the periodicity of the relation between ultrasonic attenuation and strength of magnetic field applied to a potassium crystal will be measured and from this will be derived the electron momentum at the Fermi surface. Signal generating and detection equipment is being built.

Contractor: University of Chicago

Contract Number: AT(11-1)-357

Present Contract Term: January 1, 1962 through December 31, 1962

Cost to AEC: $99,475.

Contract Title: RESEARCH ON THE SCIENCE OF MATERIALS

Investigators:
C. S. Barrett
Morrel H. Cohen
Russell J. Donnelly
David H. Douglass, Jr.
L. M. Falicov
H. Fritzsche
Robert Gomer
O. J. Kleppa
John C. Light
Donald S. Mc Clure
Lothar Meyer
Norman H. Nachtrieb
James C. Phillips
Michael G. Priestley
Ilya Prigogine
Stuart A. Rice
J. W. Stout, Jr.
Christopher B. Walker

Scope of Work: The contract between the Institute for the Study of Metals of the University of Chicago and the AEC is of a different nature from the research contracts ordinarily held by individuals. AEC funds are used specifically for the following: (1) widespread support of important general facilities utilized by all members of the Institute and other members of the University; (2) specific support of individual faculty in exploratory investigations and development of new ideas; (3) specific support of new faculty research. At the present time the funds obtained from the AEC constitute approximately 10% of the non-University contribution to the research costs in the Institute for the Study of Metals. All the research projects listed below are dependent upon and have benefited from AEC funding although in no case

have AEC funds provided full support for the project. This contract therefore is to be regarded as general support of a very broadly based research program on the science of materials. The breadth of the program is best ascertained from the topics cited below. The research cited below has also been supported by the following agencies:

Advanced Research Projects Agency
Air Force Office of Scientific Research
Army Ordnance
National Science Foundation
Office of Naval Research
United States Public Health Service

Also:

American Chemical Society
Louis Block Fund
Alfred P. Sloan Foundation
Buehler Grant

1. Structure of Uranium at Low Temperatures (C. S. Barrett)

2. Neutron Diffraction by Alpha Uranium (C. S. Barrett)

3. Strained Germanium (C. S. Barrett)

4. The Crystal Structure of Antimony at 4.2, 78 and 298°K (C. S. Barrett, P. Cucka and K. Haefner)

5. Measurements of Precise Lattice Constants (C. S. Barrett, K. Haefner and J. W. Stout)

6. Structural Studies on Cold Worked Crystalline Rare Gases (C. S. Barrett and L. Meyer)

7. Excitation Lifetime in Liquid He^3 (C. S. Barrett and L. Meyer)

8. Simultaneous Spin and Cyclotron Resonance (P. Bloomfield and M. H. Cohen)

9. Critical Points and Reflectance Spectra of Si and Ge (D. Brust and J. C. Phillips)

10. Photoelectric Yield in Si (D. Brust and J. C. Phillips)

11. Reflectance Spectra of Wurtzite Crystals (Marvin Cohen and J. C. Phillips)

12. Temperature Dependence of Semiconductor Band Gaps below the Debye Temperature (Marvin Cohen)

13. Magnetic Breakdown and Spin-Orbit Effects in Hexagonal Close Packed Metals (M. H. Cohen and L. M. Falicov)

14. Knight Shift in Superconductors (M. H. Cohen and L. M. Falicov)

15. A Study of Hydrodynamic Stability with Ion Currents (R. J. Donnelly)

16. The Effect of Modulation on the Stability Couette Flow (R. J. Donnelly)

17. The Landau Amplitude in Couette Flow (R. J. Donnelly)

18. The Periodic Boundary Layer in Hydrodymagnetics (R. J. Donnelly and D. R. Caldwell)

19. Ions in Rotating Helium II (R. J. Donnelly and D. Tanner)

20. Study of Superimposed Films of Normal and Superconducting Metals (D. H. Douglass, Jr.)

21. Surface Impedance of Metals as a Function of Magnetic Field (D. H. Douglass, Jr.)

22. Optical Constants of Sodium (Albert Feldman and H. Fritzsche)

23. Effect of Elastic Shear on Esaki Tunnel Diodes (H. Fritzsche, Gene Rochlin and J. J. Tiemann)

24. Preparation of Dislocation-Free Single Crystals of Germanium (H. Fritzsche and E. D. Dwoskin)

25. Elastoresistance of Impurity Conduction in Germanium between 1.3°K and 6°K (H. Fritzsche)

26. Intra- and Intervalley Scattering in Degenerate N-type Germanium (H. Fritzsche and M. Cuevas)

27. Impurity Conduction in Arsenic-Doped Germanium (H. Fritzsche and M. Cuevas)

28. Electrical Properties of Neutron Bombarded Germanium at Low Temperatures (H. Fritzsche and M. Cuevas)

29. The Mechanism of Superconductivity in Transition Metals (J. Garland and M. H. Cohen)

30. Complex Conductivity of Germanium as a Function of Frequency (S. Golin and H. Fritzsche)

31. Theory of Field Desorption (R. Gomer and L. W. Swanson)

32. Diffusion and Adsorption of Carbon Monoxide on Tungsten (R. Gomer, L. W. Swanson and J. Dafler)

33. Hall Coefficient in Liquid Metals and Alloys (Arthur J. Greenfield and H. Fritzsche)

34. X-ray Studies of Antiferromagnetic Compounds (Karl Haefner, J. W. Stout and C. S. Barrett)

35. Field Desorption of Hydrogen from Tungsten (B. Halpern and R. Gomer)

36. The Optical Properties of the Alkali Metals (K. P. Jain and M. H. Cohen)

37. Thermochemistry of Anion Mixtures and Reciprocal Liquid Salt Systems (O. J. Kleppa, J. M. Toguri and S. V. Meschel)

38. Anion Disorder in Monovalent Nitrates (O. J. Kleppa and F. G. Mc Carty)

39. Thermodynamics of Intermetallic Phases (O. J. Kleppa and R. C. King)

40. Thermodynamics of Liquid Metallic Solutions (O. J. Kleppa and T. Yokokawa)

41. Theoretical Chemical Reaction Rates (J. C. Light)

42. Auger Effect in Superconductive Tunneling (A. W. Luehrmann and L. M. Falicov)

43. Molecular Spectroscopy in Pulsed High Magnetic Fields (Donald S. Mc Clure)

    a. g-Factors of Excited States
    b. Spin Decoupling in Antiferromagnetic Crystals
    c. Relaxation Times for Electronic Vibrational Coupling Processes
    d. Radiationless Processes

44. Investigation of the Interactions between Ions in Crystals (Donald S. Mc Clure)

    a. Variation of Overlap of d-Orbitals with Increasing Atomic Number
    b. d-Orbital Expansion as a Function of Principal Quantum Number
    c. Measurement of Internal Fields in Magnetic Crystal by Use of Rare Earth Ion Impurity
    d. Detailed Molecular Orbital Calculations of Ion Pair Spectra
    e. Electron-Electron Decoupling Resulting from Ion Pairing
    f. Exchange Coupling between Mn^{++} Ions in ZnS:MnS

45. Charge Transport in Liquid Helium (L. Meyer and H. T. Davis)

46. Weak-Field Magnetoresistance of Hopping Conduction in Simple Semiconductors (N. Mikoshiba)

47. Strong-Field Magnetoresistance of Hopping Conduction in Simple Semiconductors (N. Mikoshiba and S. Gonda)

48. Magnetic-Field Dependence of the Acoustoelectric Effect (N. Mikoshiba)

49. Ultrasonic Attenuation by Spin of Conduction Electrons (N. Mikoshiba)

50. Ultrasonic Attenuation in Germanium (Barry Miller and H. Fritzsche)

51. Surface Tension of Metal/Molten Salt Solutions (N. H. Nachtrieb)

52. Pressure-Dependence of Self-Diffusion in Tin (N. H. Nachtrieb and C. Coston)

53. Magnetic Susceptibilities of Metals Dissolved in Molten Salts (N. H. Nachtrieb)

54. Conductance of Liquid Iondine and Solutions of Salts in Iodine (N. H. Nachtrieb and D. Bearcroft)

55. Nuclear Magnetic Resonance in Metal-Metal Salt Solutions (N. H. Nachtrieb, G. Mc Carty and S. Hafner)

56. Diffusion in Germanium at High Pressures (N. H. Nachtrieb)

57. Magnetoplasma Oscillations in Bi and Sb (R. Payne and H. Fritzsche)

58. Electronic Structure of Aperiodic Systems (D. Penn and M. H. Cohen)

59. Dielectric Screening in a Model Semiconductor (D. Penn and J. C. Phillips)

60. Dielectric Function of an "Isotropic" Insulator (D. Penn, J. C. Phillips and M. H. Cohen)

61. Interband Optical Absorption in Semiconductors (J. C. Phillips, H. Philipp and H. Ehrenreich)

62. Piezoresistance Effect in p-type Germanium (F. Pollak and H. Fritzsche)

63. de Haas-van Alphen Effect and Magnetic Breakdown (M. G. Priestley)

64. Pulsed Field Magnetoresistance of Hexagonal Metals (M. G. Priestley and J. J. Vuillemin)

65. Pulsed Field de Haas-van Alphen Studies of Semimetals (M. G. Priestley and L. Windmiller)

66. The Fermi Surface of Polyvalent Metals (M. G. Priestley and L. M. Falicov)

67. Studies of the Electronic Structure of Dense Noncrystalline Systems (S. A. Rice, M. Vala, H. Schnyders and E. G. Wilson)

    a. Vacuum Ultraviolet Reflection Spectra of Liquid Metals
    b. Electron Mobility in Simple Liquids
    c. The Properties of Dilute Liquid Metals
    d. Electronic States of Ordered and Disordered Polymeric Solids

68. Studies of the Electronic Structure of Organic Molecular Solids and Other Insulators (S. A. Rice, J. Katz, S. Choi and J. Haebig)

    a. Exciton-Exciton Interactions and Photoconductivity in Molecular Crystals
    b. The Band Structures of Excess Electrons in Organic Crystals
    c. Experimental Studies of Electron Trapping and Electron Mobility in Pure and Doped Organic Crystals
    d. Reflection Spectra of Wurtzite Class Crystals

69. Studies in Transport Phenomena (S. A. Rice, B. Lowry and L. Ikenberry)

    a. Measurement of the Viscosity of Liquid Ar, Kr and Xe
    b. Measurement of the Thermal Conductivities
    c. Extension of the Rice-Allnatt Theory to Quantum Fluids and to Mixtures

70. Studies of the Properties of Polymer Solutions (S. A. Rice, H. Yamakawa, G. Thomson and R. Corneliussen)

    a. Theoretical and Experimental Studies of the Solutions of Polar Polymers
    b. Effects of Charge and Chain Length on Friction Constants of Small Chain Molecules

71. Whisker Conductivity (L. Schmidt and R. Gomer)

72. Optical Properties of Metals and Alloys (L. G. Schulz)

73. Electron Transport in Liquid Metals (B. Springer and M. H. Cohen)

74. Magnetoplasma Oscillations and Instabilities in Electronic Conductors (B. Springer and M. H. Cohen)

75. Magnetic Anisotropy of Chlorides and Bromides of the Iron Group (J. W. Stout and DeLyle Eastwood)

76. Optical Spectra of Antiferromagnetic Fluorides (J. W. Stout and Lois Zimring)

77. Optical Properties of Antiferromagnetic Chlorides and Fluorides (J. W. Stout and S. A. Reed)

78. Magnetic Properties of Antiferromagnetic Salts (J. W. Stout and C. Trapp)

79. Heat Capacities of Antiferromagnetic Salts (J. W. Stout, S. Kim and W. Boo)

80. Vibrational Spectra of Single Crystal Fluorides of the Transition Metals (J. W. Stout and M. Steinfeld)

81. Field Desorption of Carbon Monoxide from Tungsten (L. W. Swanson and R. Gomer)

82. Transition to the Metallic State (W. D. Twose and L. M. Falicov)

83. Optical Absorption in Germanium-Silicon Alloys (W. D. Twose and J. C. Phillips)

84. Field Desorption of Ba from Tungsten (H. Utsugi and R. Gomer)

85. Field Desorption of Cs from Tungsten (H. Utsugi and R. Gomer)

86. Point Imperfections in Metals (C. B. Walker)

87. Thermal Diffuse Scattering in Powder Patterns (C. B. Walker)

88. Energy Surfaces in Magnesium in the Region of Magnetic Breakdown (Gideon Weisz and L. M. Falicov)

89. Ultraviolet Spectroscopy of Solids and Liquids (E. G. Wilson)

90. Pseudopotentials of Atoms (N. Wiser and M. H. Cohen)

91. Local Field Correction to the Dielectric Constant (N. Wiser and M. H. Cohen)

INSTITUTE FOR THE STUDY OF METALS

PUBLICATIONS, 1962

1. Allnatt, A. R. and M. H. Cohen, "Statistical Mechanics of Defect Containing Solids. I. General Formalism". Submitted to Phys. Rev.

2. Baron, Robert, "The Pressure Dependence of the NMR Chemical Shifts in Cesium and Rubidium Halides", J. Chem. Phys. (in press).

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4. Barrett, C. S., M. H. Mueller and R. L. Hitterman, "Crystal Structure Variations in Alpha Uranium at Low Temperatures", Phys. Rev. (in press).

5. Barrett, C. S., P. Cucka and K. Haefner, "The Crystal Structure of Antimony at 4.2, 78 and 298°K", Acta Cryst. (in press).

6. Birnbaum, Howard K., "Deformation Produced Point Defects--II," J. Appl. Phys. 33, 750 (1962).

7. Birnbaum, Howard K., "The Formation of Point Defects during Plastic Deformation and Their Subsequent Annealing Behavior". Submitted to J. Appl. Phys.

8. Brust, D., J. C. Phillips and F. Bassani, "Critical Points and Ultraviolet Reflectivity of Semiconductors", Phys. Rev. Lett. 9, 94 (1962).

9. Brust, D., Marvin L. Cohen and J. C. Phillips, "Reflectance and Photoemission from Si", Phys. Rev. Lett. 9, 389 (1962).

10. Caldwell, D. R. and R. J. Donnelly, "On the Reversibility of the Transition Past Instability in Couette Flow", Proc. Roy. Soc. (London) A267, 197 (1962).

11. Chisholm, R. C. and J. W. Stout, "Heat Capacity and Entropy of $CoCl_2$ and $MnCl_2$ from 11° to 300°K. Thermal Anomaly Associated with Antiferromagnetic Ordering in $CoCl_2$", J. Chem. Phys. 36, 972 (1962).

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16. Cohen, Morrel H., "Generalized Selfconsistent Field Theory and the Dielectric Formulation of the Many-Body Problem". Submitted to Phys. Rev.

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19. Corneliussen, Roger, Stuart A. Rice and Hiromi Yamakawa, "On the Thermodynamic Properties of Solutions of Polar Polymers: A Comparison of Experiment and Theory". Submitted to J. Chem. Phys.

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22. Davis, H. Ted, Stuart A. Rice and Lothar Meyer, "On the Kinetic Theory of Simple Dense Fluids. XI. Experimental and Theoretical Studies of Positive Ion Mobility in Liquid Ar, Kr and Xe", J. Chem. Phys. 37, 947 (1962).

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41. Fritzsche, H. and J. J. Tiemann, "The Effect of Elastic Strain on Interband Tunneling in Sb-Doped Germanium". Submitted to Phys. Rev.

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43. Gibbons, D. F. and L. M. Falicov, "Acoustic Measurements of the Electronic Structure of Zinc and Cadmium". Submitted to Phil. Mag.

44. Gomer, Robert and Lynn W. Swanson, "The Theory of Field Desorption". Submitted to J. Chem. Phys.

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58. Kleppa, O. J. and F. G. Mc Carty, "Heats of Fusion of the Monovalent Nitrates by High-Temperature Reaction Calorimetry". Submitted to J. Chem. Eng. Data.

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Contractor: Cincinnati, University of, Cincinnati, Ohio

Contract Number: AT(11-1)-1115

Present Contract Term: December 1, 1962 through November 30, 1963

Cost to AEC: $17,250

Contract Title: MECHANISM OF COUNTERDIFFUSION IN METALLIC SYSTEMS

Investigators: Michael Hoch and Frank R. Meeks

Scope of Work:

This program is a study of counterdiffusion and interaction of elements in the metallic state. The eventual purpose of the work is elucidation of (1) mechanism of diffusion control of solid-state reactions; (2) mechanisms of solid-state diffusion; and (3) the interplay of diffusion and interaction. Two solutions (alloys) employing a single metallic matrix ("solvent") are brought together and raised to a temperature just below the melting point of whichever alloy is lower-melting. The counterdiffusion systems studied are Al-As, Al-Sb, Ga-As, Ga-Sb, In-As and In-Sb in matrices of Cu, Ag, and Au.

It is planned to continue investigation of the mechanism of precipitate formation by X-ray analysis (in some cases, wet chemical analysis in addition) and to begin a detailed, atomic-scale study using electron-probe X-ray microanalysis.

Contractor: Clemson College, Clemson, South Carolina

Contract Number: AT(40-1)-3098

Present Contract Term: June 1, 1963 through August 31, 1964

Cost to AEC: $66,917

Contract Title: RADIATION EFFECTS IN CRYSTALLINE MATERIALS

Investigators: Robert L. Chaplin

Scope of Work:

The effects of radiation damage on solids will be investigated for single and polycrystalline materials by bombarding specimens with electrons whose energy is accurately controlled from 0.1 to 0.4 Mev by means of a Van de Graaff accelerator. Changes in physical properties by thermal annealing will be determined by the changes in resistivity, length, stored energy, or electron paramagnetic resonance. Measurements on the induced disorder in crystal structures will be used to evaluate: (1) the rate of defect production as a function of irradiation energy, (2) the threshold of atomic displacement, (3) characteristics of defect recovery, and (4) changes in structure sensitive properties per unit defect concentration. The temperature of samples during irradiation will extend from approximately $10^{o}K$ to room temperature. Pure and alloyed metals will be studied in order to assay the characteristic defect structures for various types of metallic crystals. Ionic crystals containing trace impurities will be investigated to evaluate the interaction between radiation induced defects and lattice impurities.

Contractor: Colorado School of Mines, Golden, Colorado

Contract Number: AT(11-1)-1173

Present Contract Term: May 1, 1962 through April 30, 1963

Cost to AEC: $16,918

Contract Title: STRENGTH LIMITATIONS OF METALS

Investigators: J. D. Lubahn

Scope of Work:

The objective of this project is to study the effects of size, hardness and carbon content on the notched bar strength of tempered martensitic steels. This will be done by measuring the nominal strength in concentric tensile tests of geometrically-similar notch tensile specimens throughout a practical, predetermined range of size (1/4" to 1" unnotched diameter) and carbon content (0.2 to 1.5 percent). It is believed that a definite optimum hardness, or near optimum, can be predicted for various sizes and carbon contents based on this notched bar data. The effect of alloy content, if any, will also occupy a portion of the project.

Since the following factors have been fairly thoroughly explored they will be held at appropriate values. These are the notch angle, per cent notch depth, notch profile radius, and decarburization at the root of the notch.

Also, studies are to be conducted on the optimum hardness as a function of the stress corrosion cracking strength and time for failure for austenitic stainless steels. The corrodant medium will be a chloride solution approximating the sea water. At the present time it is not known with certainty if an optimum hardness exists for coldworked stainless or whether the optimum is controlled by stress corrosion cracking. If a weakening at high hardness due to stress corrosion cracking is not observed, tests are to be conducted to determine whether there is a weakening due to other factors, such as notch brittleness.

Contractor: Columbia University, New York, New York

Contract Number: AT(30-1)-2921

Present Contract Term: February 1, 1962 through January 31, 1963

Cost to AEC: $19,710

Contract Title: SHORT CIRCUIT DIFFUSIVITY

Investigators: Eugene S. Machlin

Scope of Work:

The objectives of the researches under the proposed contract are as follows:

1. To determine the effect, if any, of normal stress on the short circuit conductivity along high angle grain boundaries in MgO. If there are positive effects, then this phenomenon will be investigated in metals using the x-ray microprobe analyzer to measure concentration profiles of boundary diffused solute and will also be further investigated in MgO to distinguish the effects of elastic stress from those of plastic deformation on the short circuit conductivity along high angle boundaries.

2. If there is a negative effect of normal stress on the short circuit conductivity along high angle grain boundaries in MgO, then an extended study will be made to determine the effect of the magnitude of the Burgers vector on the short circuit diffusivity along isolated dislocations in various metals using the x-ray microprobe analyzer to detect such diffusion.

3. To measure quenched-in residual resistivities and their annealing out kinetics in vertical zone-refined copper, iron, tungsten using the controlled atmosphere quenching-in apparatus.

Contractor: Connecticut, University of, Storrs, Connecticut

Contract Number: AT(30-1)-2047

Present Contract Term: April 15, 1962 through April 14, 1963

Cost to AEC: $39,800

Contract Title: INVESTIGATIONS OF RADIATION EFFECTS IN SOLIDS BY ELECTRON SPIN RESONANCE

Investigators: O. R. Gilliam

Scope of Work:

Single crystals of metal oxides and metal azides are being investigated by electron spin resonance (ESR) for radiation-induced changes in their paramagnetic defect structure. An electron Van de Graaff accelerator, the Brookhaven Research Reactor, gamma sources and ultraviolet lamps are used for the irradiations. Materials upon which investigations are being conducted are aluminum oxide, titanium dioxide, fused silica, potassium azide and sodium azide. The major objectives of the research is to study the growth and stability of the various radiation-induced defects, to identify these defects, to correlate the induced spin resonance absorptions with other radiation damage phenomena, and to find wave functions and methods of predicting the ESR optical characteristics of the paramagnetic centers.

At least five different paramagnetic centers caused by various radiations are found in aluminum oxide, all of which appear to be hole-like in character. The absence of hyperfine structure increases the problem of the identity of these centers; however, symmetry properties and fine structure characteristics have enabled some tentative assignments to be made.

A report on several centers in potassium azide exhibiting hyperfine interactions with a N^{14} nucleus or with N^{14} nuclei has been published previously. Further studies of these centers in potassium azide and some centers in sodium azide which may be similar are in progress.

A theoretical investigation of the relationship of the F-center defect structure in the alkali halides to that in the alkali azides has been initiated.

Spin resonances generated in TiO_2 by gamma-ray irradiations at $77^{\circ}K$ and changes in the valence states of impurity ions are being examined to learn the source of the energy levels in the semi-conducting rutile.

Recent Publications:

D. W. Wylie, A. J. Shuskus, C. G. Young, O. R. Gilliam and P. W. Levy, "Electron Spin Resonance of Radiation-Induced Defects in Potassium Azide," Phys. Rev. 125, (1962).

Contractor: Cornell University, Ithaca, New York

Contract Number: AT(30-1)-1994

Present Contract Term: June 1, 1962 through May 31, 1963

Cost to AEC: $12,334

Contract Title: LIQUID-SOLID INTERFACIAL TENSIONS IN METAL ALLOY SYSTEMS

Investigators: C. W. Spencer

Scope of Work:

The kinetics of liquid film penetration into grain boundaries in oriented bi-crystals of nickel is being studied as a function of relative crystallographic orientation, temperature, and direction upon the boundary surface. In general, a parabolic rate law, $x = \sqrt{kt}$, relating distance penetrated to time of penetration is observed. In bi-crystals possessing a 42° tilt orientation about <100> , subjected to liquid bismuth, the rate of penetration is found to be anisotropic with the direction of penetration into the boundary, the rate in the direction perpendicular to the <100> being greater. The thermal activation can be expressed by the Arrenhius equation, $k_{\perp} = 0.6 \exp(-36{,}000/RT)$ and $k_{\parallel} = 1.0 \exp(-42{,}000/RT)$ cm^2 sec^{-1}.

Recent Publications:

F. C. Hochgraf and C. W. Spencer, and R. F. Cheney, "Penetration of Liquid Bismuth into the Grain Boundaries of a Nickel Alloy," AIME Trans., 221, (1961) p. 492.

R. J. Knight, Che-yu Li, C. W. Spencer, "Monotectic Reaction in the Bismuth-Selenium System," Submitted to AIME Trans.

G. H. Bishop, B. F. Addis, C. A. Steidel, C. W. Spencer, "Liquid Bismuth Penetration into Oriented Bicrystals of Nickel," Submitted to AIME Trans.

Contractor: Cornell University, Ithaca, New York

Contract Number: AT(30-1)-2150

Present Contract Term: April 1, 1962 through March 31, 1963

Cost to AEC: $92,535

Contract Title: SOLID STATE PHYSICS: MAGNETIC PHENOMENA

Investigators: Raymond Bowers and R. H. Silsbee

Scope of Work:

Scope I: Electron Spin Resonance Work

Two articles were published recently, one dealing with the identification of a defect produced by neutron irradiation of crystalline quartz and the other describing a detailed study of the changes in the spin resonance and optical properties of additively colored KCl induced by optical bleaching of the F-band. Current studies include a detailed study of the F-center resonance by a double microwave resonance technique and an investigation of the effect of cation vacancy motion on the relaxation time of the F spin resonance. Transition element impurities are the subject of two experiments, one involving electric field effects, the other entailing a search for a long-range phonon coupled interaction between spins. A final experiment is the search for anomalous Knight shifts in small metal particles.

Scope II: Magnetic Phenomena and Electronic Structure

The following topics have been investigated during the past year and are being continued this year. (a) The study of C.C. magnetoresistance of sodium and lithium. (b) A study of the excitation of magneto-plasma modes in the electron gas of sodium. (c) Collaboration with the Chalk River group on the study of the phonon spectra of sodium using neutron scattering methods. (e) Growth of single crystals of sodium and lithium.

Recent Publications:

R. Bowers, C. Legendy, F. Rose, "An Oscillatory Galvano-Magnetic Effect in Metallic Sodium," Phys. Rev. Ltrs. 7, (1961) p. 339.

A. D. B. Woods, B. N. Brockhouse, R. H. March, and R. Bowers, "Normal Vibrations of Sodium," Proc. Phys. Soc. (1961) In press.

R. Bowers, D. Pinnow, and S. Tallman, "Single Crystals of Lithium and Sodium 1961. Report # 3," The Materials Science Center, Cornell University.

R. H. Silsbee, "Electron Spin Resonance in Neutron-Irradiated Quartz," Journal Appl. Phys. 32, (1961) p. 1459.

P. R. Moran, S. H. Christensen, and R. H. Silsbee, "Electron Spin Resonance and Optical Absorption of Electron Excess Centers in KCl," Phys. Rev. 124, (1961), p. 442.

Contractor: Cornell University, Ithaca, New York

Contract Number: AT(30-1)-2391

Present Contract Term: April 1, 1962 through March 31, 1963

Cost to AEC: $138,689

Contract Title: SOLID STATE PHYSICS: TRANSPORT AND RELATED PHENOMENA

Investigators: R. L. Sproull and J. A. Krumhansl

Scope of Work:

Scope I: Low-Temperature Thermal Conductivity (R. O. Rohl and R. L. Sproull)

This research has as its purpose the study of phonon defect interactions in non-metallic crystals, primarily by use of thermal conductivity measurements and their analyses. KCl doped with KNO_2, KI and other defects has been the material usually used. A variety of optical, chemical and electronic techniques are used in conjunction with these studies.

Scope II: Theoretical (Phonon) Physics (P. Carruthers and J. A. Krumhansl)

Comprises both solid state theory and its application to thermal conductivity and lattice vibration and general field of theoretic and many-body physics. Phonon scattering, localized lattice vibrations and resonance mechanisms and thermal conductivity are under study. Pion and pion nucleon scattering theory is also being investigated.

Recent Publications:

M. V. Klein, "Phonon Scattering in Sodium Chloride Containing Oxygen," Phys. Rev. 122, (1961) p. 1393.

M. V. Klein, "Effects of Precipitation of Dissolved $MnCl_2$ on Low Temperature Thermal Conductivity of NaCl," Phys. Rev. 123, (1961) p. 1977.

P. Carruthers, "Resonance in Phonon-Phonon Scattering," Phys. Rev. 125, (1962) p. 123.

P. Carruthers, "Integral Equations for the Process $3_\pi - 3_\pi$," Nuovo Cimento 22, (1961) p. 867.

P. Carruthers, "Thermal Conductivity of Solids III; Iso-anharmonic Effect," Submitted to Phys. Rev.

J. A. Krumhansl, "Thermodynamics of Energy Conversion Systems," Enrico Fermi Summer School Supplemento al Nuovo Cimento, In press.

J. A. Krumhansl, "Lattice Vibrations in Solids," Journal Appl. Phys. In press.

Contractor: Cornell University, Ithaca, New York

Contract Number: AT(30-1)-2471

Present Contract Term: October 1, 1962 through September 30, 1963

Cost to AEC: $56,600

Contract Title: STUDY OF IMPERFECTIONS IN CRYSTALS BY MEANS OF INTERNAL FRICTION MEASUREMENTS

Investigators: H. S. Sack

Scope of Work:

In an attempt to clarify the origin of the Bordoni-type internal friction peaks at low temperatures in plastically deformed crystalline materials, the measurements were extended to bcc and hexagonal metals and to fcc ionic crystals. It appears that the peaks observed in the different crystallographic systems show characteristic differences, e.g., in the variation of height and temperature with amount of cold work and annealing. In ionic crystals there are indications that charged dislocations play a role.

All peaks show a structure: Studies of samples deformed at low ($4^{\circ}K$) temperature permit a sharp resolution of this structure and suggest that it is caused by the activation of several slip systems. This view is supported by the variation of the peak width with peak temperature, which shows that the width is caused by a distribution of activation energies (possibly in combination with a distribution of attempt frequencies).

It is planned to continue the study of these peaks, complemented in the case of ionic crystals by dielectric measurements, in order to elucidate the properties of dislocations and their interactions with point defects.

Study of surface effects and imperfections on the trapping of electrons and holes in AgCl is being continued.

Recent Publications:

A. Taylor, "Low Temperature Internal Friction Peaks in Single Crystals of NaCl and LiF. Journal of Applied Physics, 32, 1799

D. A. Wiegand, "Photo Impedance of the AgCl Electrode System" Phys. Review, 124, 104 (1961)

Recent Publications:

A. Taylor, "Low Temperature Internal Friction Peaks in Monocrystalline LiF. Acta Met. 10, 490 (1962).

R.T.C. Tsui and H. S. Sack, "Internal Friction in Plastically Deformed Magnesium. Bull. Am. Phys. Soc. 7, 224 (1962)

Contractor: Cornell University, Ithaca, New York

Contract Number: AT(30-1)-2504

Present Contract Term: February 1, 1963 through January 31, 1964

Cost to AEC: $41,000

Contract Title: A STUDY OF RATE-CONTROLLING PROCESSES IN DEFORMATION

Investigators: Arthur L. Ruoff

Scope of Work:

During the past year the activation volumes and energies for the creep of lead have been measured. These values are in essential agreement with the corresponding values for self-diffusion, leaving little doubt that the diffusion of vacancies, from very slight vacancy supersaturations at the sources, to the sinks is the rate-controlling process in high temperature creep (strain rates up to 10^{-4} sec^{-1}) of lead and probably other face centered cubic metals as well. Similar measurements have also been carried out in aluminum, and we are now studying the pressure dependence of vacancy motion in aluminum by nuclear magnetic resonance as well.

Special attention has been focused on the temperature and pressure dependence of creep in the alkali metals. In sodium and potassium we have found that for low strain rates the results are in very good agreement with the self-diffusion values so that again vacancy motion is the likely mechanism. For high strain rates both the activation energy and volume are almost doubled. The results are completely consistent with crowdion formation at those sites which normally act as vacancy sinks if the crowdion is the stable interstitial type defect. Calculations on the crowdion stability are underway. Experimental work over a larger temperature range is also in progress. In addition, we are doing work on single crystal materials. We will also make measurements on cesium and rubidium.

We have extended our pressure range to 18 kilobars; we can very conveniently measure creep under these conditions using a system which can be accurately calibrated in situ. We are using such a system to measure the pressure dependence of the activation volumes in the alkali metals and to extend our work on bismuth, which shows nearly a zero activation volume, to the region in which a phase change occurs.

Recent Publications:

R. H. Cornish and Arthur L. Ruoff, "Electrical Leads for Pressure Vessels to 30 Kilobars", Rev. Sci. Inst. 32 639 (1961).

B. M. Butcher and A. L. Ruoff, "Effect of Hydrostatic Pressure on the High-Temperature Steady-State Creep of Lead," J. Appl. Phys. Oct., 1961.

Contractor: Cornell University, Ithaca, New York

Contract Number: AT(30-1)-2558

Present Contract Term: April 15, 1962 through April 14, 1963

Cost to AEC: $15,569

Contract Title: SOLIDIFICATION REACTIONS

Investigators: H. W. Weart

Scope of Work:

The mechanism of formation of cellular (non-planar on a macroscopic scale) solid-liquid eutectic interface is being studied experimentally by determining the distribution coefficients (k) of major components and impurities between several metallic eutectics and their melts. Within experimental error, the major components of Cd-Sn, Cd-Zn and Bi-Cd eutectics have k's equal to one. In the Sn-Zn eutectic, the k for Zn appears to be well below one. Since microstructural changes accompany composition changes along the unidirectionally solidified bars, this system is being studied further to determine if nucleation effects are involved.

Impurities are observed to have k's different from one, as anticipated, but measurements of these k's by use of tracers are not complete.

A theoretical analysis of eutectic solidification is being made by using the thermodynamics of irreversible processes. The first result was the following relation between interlamellar spacing, S, and growth velocity, v, in a highly idealized and simplified eutectic model: $S\,v = \text{constant}$. This functional relation between S and v has been tested experimentally in one eutectic, and the relation appears valid at very small values of v. A more realistic model is now being examined.

Contractor: Cornell University, Ithaca, New York

Contract Number: AT(30-1)-3029

Present Contract Term: June 1, 1962 through May 31, 1963

Cost to AEC: $87,325

Contract Title: HARD SUPERCONDUCTING MATERIALS

Investigators: J. Silcox and W. W. Webb

Scope of Work:

This program is aimed at elucidating the effects of dislocations and other defects on characteristic superconducting properties including critical current, critical field curves. Study of the defects will be carried out by transmission electron microscopy, x-ray diffraction topography and standard metallographic procedures. Cryogenic equipment for measuring supercondicting properties is at present either in the process of construction or already in operation. Initial experiments will be carried out to follow two main approaches:

(a) To determine the arrangement and movement of dislocations in an attempt to correlate this with the superconducting properties. It is hoped to grow single crystals of Nb_3Sn and Pb_3Bi suitable for work in this area with x-ray diffraction topography. Work will also be carried out on Nb and Ta using transmission electron microscopy.

(b) To determine the extent to which various types of disorder control the superconducting properties. Thus it is planned to compare the superconducting properties of Nb after irradiation and after deformation.

Contractor:	Cornell University, Ithaca, New York
Contract Number:	AT(30-1)-3087
Present Contract Term:	September 1, 1962 through August 31, 1963
Cost to AEC:	$42,740
Contract Title:	CORRELATION OF PHYSICAL PROPERTIES OF CRYSTALS WITH MICROSTRUCTURE
Investigators:	John Silcox

Scope of Work:

The emphasis at this stage of the program will be on the correlation of the magnetic properties of nickel with microstructure as revealed by transmission electron microscopy. A vibrating magnetometer presently being built will be utilized to make measurements of the coercivity of specimens of nickel deformed to various levels. Observations of the dislocation structure will be made by electron microscopy and an attempt will be made to verify Vicena's theory. Similar experiments will be carried out on nickel containing nonferromagnetic precipitates and quenched and irradiated nickel. It is also planned to make electrical resistivity measurements on these specimens simultaneously with the observations on magnetic properties. It is likely that experiments will be carried out on single crystals. These experiments are directly related to the interaction of magnetic domain walls with various microstructural features. It is also planned to initiate work on the nucleation of magnetic domains on cooling past the Curie point.

Contractor: Cornell University, Ithaca, New York

Contract Number: AT(30-1)-3228

Present Contract Term: June 7, 1963 through June 6, 1964

Cost to AEC: $30,615

Contract Title: SOLID-LIQUID INTERFACE

Investigators: Che-Yu Li

Scope of Work:

From the kinetic data of grain-boundary grooving in the presence of a saturated liquid the solid-liquid interfacial tension can be calculated. Experiments have been designed to study by this method, the temperature and concentration dependence of solid-liquid tension so that the surface entropy and surface concentration can be determined separately to allow further theoretical analysis.

Two systems have been chosen for study: a) grain boundary grooving in Nb bicrystals by liquid Li and b) edge rounding of LiF crystals by H_2O containing varying amounts of HF.

Contractor:	Delaware, University of, Newark, Delaware
Contract Number:	AT(30-1)-2722
Present Contract Term:	February 1, 1963 through January 31, 1964
Cost to AEC:	$36,640
Contract Title:	STATISTICAL THERMODYNAMICS OF METALLIC SOLUTIONS
Investigators:	Leonard P. Skolnick

Scope of Work:

An improved computer program has been developed to obtain thermodynamic data for ternary systems from integral data or partial data from one of the components. We are presently working on the statistical basis for testing theoretical expressions in such a way that the statistical validity of various linear terms may be independently obtained.

Theoretical work has been primarily concerned with fitting a Morse-type potential into conformal solution theory. No progress has so far been made in the more ambitious goal of putting an electronic theory directly into the original statistical mechanical model.

Experimentally we have emphasized work on the system Cu-Au-Ag. A Knudsen cell apparatus has been constructed for thermodynamic measurements in the Ag-rich corner and EMF equipment is almost completed for the study of Cu-rich alloys.

Initial work function measurements on Cu-Au-Ag alloys should be made in the near future. The work function apparatus is under test now, making measurements of the work function of Tantalum.

Nuclear magnetic resonance equipment has been modified and the spectra of Cu-Au alloys is being studied. Concurrently a new X-ray technique for measuring the effective Debye temperature of these alloys is being developed.

Contractor:	Denver, University of, (Colorado Seminary), Denver, Colorado
Contract Number:	AT(11-1)-1298
Present Contract Term:	June 1, 1963 through May 31, 1964
Cost to AEC:	$26,170
Contract Title:	ALLOYING BEHAVIOR OF THE RARE EARTHS
Investigators:	J. F. Nachman and C. E. Lundin

Scope of Work:

Rare earth binary alloy systems are to be used to study the effects of simple variables on phase relations and thermodynamic activity. The rare earths are useful for such an investigation because of the many similarities among the characteristics of the rare earth elements and the slow change in such properties as atomic size as one progresses across the rare earth period.

Past research at Denver on the Nd-Pr diagram has shown that the solutions in this system are essentially ideal, as would be predicted by the similarity of the atoms of these two elements. The present program will extend this investigation into systems in which the species differ in one or two of their characteristic properties. The first two systems to be studied are the Sm-Gd and Y-Gd binaries.

Contractor:	Emory University, Atlanta, Georgia
Contract Number:	AT(40-1)-2953
Present Contract Term:	January 1, 1963 through December 31, 1963
Cost to AEC:	$9,913
Contract Title:	THE DETERMINATION OF LOW ENERGY X-RAY ABSORPTION COEFFICIENTS
Investigators:	Robert H. Rohrer and Randall W. Carter

Scope of Work:

The Contractor will determine X-ray absorption coefficients for light elements, including Ni, Zn, Cu, Co, Fe, Cr, Al, and Mg, in the energy region below 6 Kev. Methods of thin film target production, evaluation, and handling will be investigated. Theoretical equations for mass absorption coefficients as a function of energy will be proposed. The mechanism of the attenuation of low-energy X-rays by matter will be studied.

Contractor: Florida, University of, Gainesville, Florida

Contract Number: AT(40-1)-2581

Present Contract Term: June 1, 1962 through May 31, 1963

Cost to AEC: $32,827

Contract Title: TOPOLOGICAL STUDY OF THE SINTERING PROCESS

Investigators: F. N. Rhines and John Kronsbein

Scope of Work:

The object of this research is the determination of the fundamental factors involved in determining the sintering behavior of three dimensional aggregates. Areas of concern are: a) attempts to extend and generalize the theory of quantitative metallography, b) measurements of the genus, surface area, specific volume, curvature and pore size distribution for a variety of powders and environments, c) the search for interrelations among the various geometric variables, d) investigations of the kinetics of the four geometric processes that occur during sintering (densification, surface rounding, channel closure, and pore segregation), and e) measurements of the force of sintering as a function of starting material and environment.

Recent Publications:

F. N. Rhines, "Rate of Densification in the Sintering of Uncompacted Metal Powders," Interscience, (1962) p. 351. Int'l. Symposium on Agglomeration.

F. N. Rhines, "Size Sensitivity in the Two Particle Case," Plansee Proceedings, (1961).

F. N. Rhines, "Determination of the Size Distribution of Ellipsoidal Particals from Measurements Made upon Random Plane Sections, Accepted for publication, Trans. AIME, (1962).

Contractor: Florida, University of, Gainesville, Florida

Contract Number: AT(40-1)-2857

Present Contract Term: November 1, 1962 through August 31, 1963

Cost to AEC: $16,114

Contract Title: THE NATURE OF ATOMIC BINDING IN DILUTE SOLID SOLUTIONS

Investigators: Albert G. Guy

Scope of Work:

The laboratory work that will be done can be listed under the following headings: a) preparation of floating-zone refined, iron-base solid solutions; b) construction of a precision instrument for measuring thermal expansion at low temperatures; c) measurement of thermal expansion on high-purity iron and its solid solutions at liquid hydrogen and liquid helium temperatures using the above instrument, and at higher temperature using the Leitz dilatometer; d) measurement of electrical resistivity on high-purity iron and its solid solutions at liquid hydrogen and liquid helium temperatures; e) measurements of elastic properties and studies involving nuclear resonance may also be made by other staff members in view of the availability of the interesting high-purity alloys.

The results obtained will be correlated with existing data on these phenomena, and an attempt will be made to fit them into a theoretical structure.

Recent Publications:

A. G. Guy, "Acceleration of Deformation by Concurrent Phase Change" Trans. Met. Soc. AIME, 221 (1961) pp. 802-807.

A. G. Guy, "Effect of Strain on Diffusion in Metals," Trans. Met. Soc. AIME, 221 (1961) pp. 1174-1178.

A. G. Guy, "Pourbaix Diagrams - A Firm Basis for Understanding Corrosion," Metal Treatment, February, 1962.

A. G. Guy, "Structural Changes Accompanying the Formation of the K-State" ASM Transactions Quarterly, September, 1962.

Contractor:	Franklin Institute Laboratories, Philadelphia, Pennsylvania
Contract Number:	AT(30-1)-2730
Present Contract Term:	January 15, 1962 through January 14, 1963
Cost to AEC:	$30,000
Contract Title:	SOLID STATE INVESTIGATIONS UTILIZING ELECTRON-BOMBARDMENT PHENOMENA
Investigators:	Martin A. Pomerantz

Scope of Work:

The purpose of this work is to utilize high energy electron bombardment as a tool for investigating certain properties of solids. Relevant theoretical studies are also contemplated.

Measurements of the energy-dependence of the secondary electron emission from various metals is undertaken. Bombardment-induced conductivity, and post-bombardment conductivity of magnesium oxide will be measured over a wide temperature range. Other experiments, such as determinations of the thermoelectric power and the Hall effect of bombarded MgO crystals will be conducted. The experimental techniques for investigating the properties of solids will be extended to include other crystals, if time permits.

Contractor: Franklin Institute Laboratories, Philadelphia, Pennsylvania

Contract Number: AT(30-1)-2994

Present Contract Term: March 1, 1962 through February 28, 1963

Cost to AEC: $114,300

Contract Title: SOLID STATE RESEARCH

Investigators: H. G. F. Wilsdorf

Scope of Work:

Task I The atomistic distribution and the behavior of lattice defects in metal crystals exposed to pile neutrons are studied by transmission electron microscopy and other experimental techniques. Copper and nickel are affected differently by comparable exposures. The nucleation and growth of point defect clusters as well as the resulting lattice defects are investigated in order to explain the observed differences.

Task II The static lattice distortions around interstitial atoms, chemically introduced into the host lattice, are measured by intensity changes, lattice parameter changes and diffuse x-ray scattering. For oxygen in titanium good agreement was obtained between the observed intensity reduction and that calculated using the experimental variation of the lattice parameter with concentration.

Task III Surface diffusion measurements utilizing radioactive tracers are being made on oriented surfaces of face-centered cubic metals. Activation energies are determined, and the effects due to annealing atmospheres and the contributions of volume diffusion at elevated temperatures are studied. Pertinent theoretical treatments of simultaneous surface and bulk migration are developed.

Task IV Metallic films are made by evaporation in ultra high vacuum at different temperatures and in the presence of adsorbable gases. Perfection and annealing behavior of the crystallities constituting the film are measured by x-ray diffraction as a function of gas pressure and temperature without removing the specimen from the vacuum chamber.

Contractor:	General Mills, Inc., Mechanical Division Minneapolis, Minnesota
Contract Number:	AT(11-1)-722
Present Contract Term:	February 15, 1963 through February 14, 1964
Cost to AEC:	$57,187
Contract Title:	SURFACE BOMBARDMENT STUDIES
Investigators:	Gottfried K. Wehner

Scope of Work:

There are two primary areas of work in this program, the sputtering of single crystals and sputtering yield measurements with mass separated hydrogen beams.

The sputtering of single crystals by ion bombardment generally results in a pronounced atom ejection in certain preferred directions. The interpretation of these atom ejection anisotropies is invaluable for a basic understanding of the sputtering mechanism and of radiation damage. Information is obtained, for instance, on what types of correlated collision sequences are operative and their relative importance in various crystals. These results also give information on the presence of interstitials near the surface and the location of surface atoms which are not in normal lattice positions.

Sputtering yields for H_1^-, H_2^-, and H_3^- are being determined for various target metals and bombarding energies from measurements of the time taken by beams of these ions to pierce holes in target foils. Such data are of importance in thermonuclear fusion devices as well as in "solar wind" bombardment and radiation damage problems.

Recent Publications:

G. S. Anderson, "Atom Ejection in Low Energy Sputtering of Single Crystals of fcc Metals and of Ge and Si," Journal of Appl. Phys., Vol. 33, No. 6, (1962) pp. 2017-2025.

G. S. Anderson, "Atom Ejection in Low Energy Sputtering of Single Crystals of bcc Metals," Submitted to Journal of Appl. Phys.

Contractor: Georgia Institute of Technology, Atlanta, Georgia

Contract Number: AT(40-1)-2755

Present Contract Term: June 1, 1962 through May 31, 1963

Cost to AEC: $64,714

Contract Title: SURFACE PROPERTIES OF MAGNETIC MATERIALS

Investigators: Edwin J. Scheibner

Scope of Work:

The purpose of the research in progress under this contract is to investigate various properties of the surfaces of magnetic materials. During the previous two years under this contract four types of studies were made. 1) Equipment and techniques for preparing high purity magnetic films were developed. 2) A torsion magnetometer was constructed and preliminary measurements were made of the magnetization of thin nickel films as a function of temperature. 3) Concurrent with these studies other nickel films were prepared in an ultra-high vacuum system and subsequently oxidized. During the preparation and oxidation the magentic characteristics were monitored with a sensitive hysteresis loop tracer. 4) The initial attack of CO on stainless steels was studied by transmission electron microscopy of electrolytically thinned specimens. In the proposed research these four studies will be continued.

Contractor:	Harvard University, Cambridge, Massachusetts
Contract Number:	AT(30-1)-1956
Present Contract Term:	September 1, 1962 through August 31, 1963
Cost to AEC:	$66,290
Contract Title:	REACTIONS BETWEEN SOLID AND LIQUID METALS AND ALLOYS
Investigators:	Bruce Chalmers

Scope of Work:

This research is a continuation of our study of the processes that take place at solid-melt interfaces and control the processes of melting and of solidification. The particular aspects at present under investigation are: 1) the origin and detailed morphology of the substructures that occur in crystals grown from the melt, 2) study of the physical parameters that control the morphology of eutectics and peritectics, 3) the inclusion or rejection of solid particles by an advancing solid-liquid interface. In each case, a theoretical study is being conducted in association with the experimental program.

Contractor:	Houston, University of, Houston, Texas
Contract Number:	AT(40-1)-2573
Present Contract Term:	February 1, 1963 through January 31, 1964
Cost to AEC:	$53,720
Contract Title:	SPUTTERING BY ION BOMBARDMENT
Investigators:	H. K. Reynolds and J. C. Allred

Scope of Work:

The program concerns the investigation of various materials under bombardment of heavy ion beams. The rates of sputtering of various target materials are measured as a function of the energy and nature of the bombarding ion, its angle of incidence on the target. The energy range investigated is 20 Kev to 200 Kev. Materials to be investigated are both polycrystalline metals and mono-crystalline metals, and non-metals. The method of measurement is to collect the sputtered atoms on nearby surfaces and measure the thickness of the collected layer. Three methods are in use or proposed. 1) Multiple Beam Interferometry on glass collector plates, 2) Optical density measurements on glass plates, calibrated against the Interferometer measurements, and 3) Collection on a quartz crystal and measuring the change in frequency of the oscillator due to the increased mass. Measurements on a single crystal target will investigate the dependence of yield on crystal direction and the relation between crystal axes and bombarded surface. Theoretical investigations of the sputtering mechanism will also be made, with particular attention to the relation between sputtering angular distribution and the crystal axes directions.

Contractor: Illinois, University of, Urbana, Illinois

Contract Number: AT(11-1)-1046

Present Contract Term: June 1, 1962 through May 31, 1963

Cost to AEC: $26,700

Contract Title: MECHANICAL BEHAVIOR OF DILUTE ALLOYS OF NIOBIUM

Investigators: G. M. Sinclair

Scope of Work:

This program is being carried out cooperatively between the Department of Mining and Metallurgical Engineering and the Department of Theoretical and Applied Mechanics. It involves studies of metallurgical control of composition of dilute niobium alloys and their mechanical behavior over a wide range of temperatures.

Metal gas equilibria and the niobium-nitrogen and niobium-oxygen terminal solid solutions are being studied. The niobium-nitrogen binary is found to obey the rules for ideal behavior very well and as a result the major features of the binary may be described by a small number of thermodynamic parameters.

The yield behavior of polycrystalline niobium is being studied in the temperature range 78°K to 400°K and at strain rates differing by six orders of magnitude. It is found that rate and temperature dependence of the yield stress can be described by a stress-dependent activation energy relation. Work is continuing on niobium single crystals.

Contractor: Illinois, University of, Urbana, Illinois

Contract Number: AT(11-1)-1198

Present Contract Term:

Cost to AEC: $1,150,000 (Fiscal year 1963)

Contract Title: THE SCIENCE OF MATERIALS

Investigators: R. J. Maurer (Acting for F. Seitz) and Associates

Scope of Work:

This master contract embraces the following projects many of which were previously independent contracts.

I. Very Low Temperature Properties of Solids

A. Properties of Rare Gas Solids - R. O. Simmons

This project aims to study large single crystals of neon, argon, krypton and xenon. Specifically it aims to develop techniques for manipulation of such crystals to verify directly their crystalline perfection by x-ray diffraction techniques, to measure as a function of temperature their lattice constants, their thermal expansivity, their isothermal compressibility and the intensities of selected Laue-Bragg diffraction maximum. These data will be compared to measurements of other thermodynamic properties and to existing theories of crystal lattice dynamics. Particular emphasis will be placed upon the temperature interval between 2 and 30°K for which few data exist. A study of zero point and anharmonic effects will be focused on isotopically pure Ne^{20} and Ne^{22} crystals.

B. Research on the Properties of Materials at Low Temperatures - J. C. Wheatley

The purpose of this program is to study the properties of materials at very low temperatures. Currently, the work is devoted entirely to He^3. At temperatures below 0.01 K a search is being made for a highly correlated phase of liquid He^3 which has been predicted from the BCS theory by several theoreticians. Furthermore at these temperatures, the phenomena of propagation of zero sound as predicted by Landau is being sought. An attempt will be made to determine more accurately the limits of validity of and the parameters for the Fermi liquid theory as applied to liquid He^3. The experimental approach used will be dictated by the results of work under way at present on refrigeration and thermal isolation technique. The most likely properties of He^3 to be measured are the diffusion coefficient, the magnetic susceptibility, the thermal diffusivity and the velocity and attenuation of sound.

Plans are also being made to make quantitative studies of He^3 at presently assessible temperatures, that is above .01°K. These include measurements of the attenuation of sound, the thermal diffusivity and the thermal boundary resistance between liquid He^3 and a solid.

II. Intrinsic Structure and Properties of Solids

A. Electronic Specific Heat Study of the Alloys of Transition Elements
P. A. Beck

The electronic specific heat of b.c.c. alloys of 3d transition elements alloyed with non-transition elements such as aluminum will be measured as a function of electron concentration. Similar studies will be made with b.c.c. alloys of 4d and 5d transition elements with one another. Low temperature specific heat measurements will be made in a magnetic field with superconductive alloys of the Ti-V system.

Past results indicate that the electronic specific heat of alloys of transition elements with one another can be described in terms of a more or less rigid band; the degree of filling of this band being determined by the average electron concentration of the alloy. Such an explanation of the specific heat data of alloys involving non-transition elements such as Al, Sn, and Sb does not seem possible. The effects of non-transition elements on the shape of the d-band is being determined by studying the electronic specific heat of alloys over a relatively wide range of electron concentration with fixed amounts of non-transition element additions.

A study of b.c.c. solid solutions in the systems Zr-Nb, Nb-Mo, and Mo-Re is contemplated. In the Ti-V alloy system, the critical magnetic field vs. superconductivity transition temperature relation will be measured.

B. High Pressure Studies of Inter- and Intramolecular Forces - H. G. Drickamer

The purpose of this project is the investigation of intermolecular and intramolecular forces, using high pressure as a tool for varying interatomic distance. Present and future studies include: (1) Optical studies to 170 kb of pi-electron spectra in fused ring aromatic compounds and in complexes. The effects of interatomic distance on the perturbation of molecular spectra, on charge transfer, and on Davydov splitting are included. (2) Electrical resistance measurements to 600 kb. Studies include the approach to the metallic stage in valence, ionic, and molecular crystals, and electronic rearrangements, especially in the alkali, alkaline earth, and rare earth metals.

Techniques are being developed for several new kinds of measurements at high pressure. It appears possible to make x-ray measurements of interatomic distance to at least 400 kb. These measurements will be of the utmost importance for theoretical work. Initial investigations indicate that Mössbauer studies to perhaps 200 kb are feasible. Efforts are in progress to develop a technique to permit NMR studies to 50 kb.

C. Low Temperature Thermal Conductivity Studies - M. V. Klein

Apparatus for the measurement of thermal conductivity has been designed and is about ninety-five percent assembled. An NRC crystal-growing furnace has been delivered and is in the process of assembly. Research should be under way in this area very shortly.

Infrared and ultraviolet absorption measurements have been made on NaCl, NaBr, KCl and KBr doped with OH^-. The strengths of the absorption bands observed are being calibrated by chemical determinations of the OH content. This work will act as a foundation for the thermal conductivity work on the OH^- doped halides but it is also complete in itself.

A theoretical calculation has been made of the effect of the zero-point-induced strain field around a He^3 atom in solid He^4 on the phonon scattering. Furthermore, theoretical work has been started in the general area of resonance scattering of phonons by pseudo-localized lattice modes.

This project will continue the present work on the low temperature thermal conductivity of insulators (phonon conductivity). The work will be extended to include not only measurements on chemically produced defects but also defects produced photochemically by x-rays. Of particular interest will be the role played in phonon scattering by the anti-alpha center, the presumably interstitial center that is the partner to the alpha center (negative ion vacancy) in alkali halides. The first measurements to be made will be on alkali halides doped with hydroxide and on mixed crystals such as NaCl:K, NaCl:Ag and NaCl:Br. In addition to the experimental work, theoretical work in the general area of resonance scattering of phonons by pseudo-localized lattice modes will be performed.

D. Dielectric and Structural Investigation of Complex Compounds of the Perovskite Type ABO_3 - V. J. Tennery

The purpose of this project is an investigation of the dielectric and other electrical properties of complex compounds having the Perovskite structure and the chemical formula ABO_3 where not all of the A cations are of the same type. It is hoped that the investigation will shed light on the conditions that determine the occurrence of ferroelectricity and antiferroelectricity in oxide structures since rather extensive ionic substitutions can be made without catastrophic changes in crystal structure.

The investigation will be concerned primarily with the determination of the conditions for the formation of compounds such as $A_1^{+1}((B_1^{+6})_{3/4}(B_2^{+2})_{1/4})O_3$ and the examination of their real and complex permitivities. Those compounds that are found to be ferroelectric will be studied as single crystals if they can be grown by conventional techniques.

Crystal symmetry and lattice parameters will be investigated by conventional x-ray techniques.

E. Nuclear Magnetic Resonance Studies - T. J. Rowland

It is the objective of this project to study the electronic structure of metals as revealed by nuclear magnetic resonance. Specific studies will be made of dilute silver alloys in an attempt to resolve certain fine structure in the Knight shift. Also, searches will be carried out for nuclear resonances not yet observed in metals. If the latter are successful, work may be initiated on alloys of these metals. Exploratory investigations of radiation damage and of temperature and pressure dependence of the shift due to the conduction electrons will also be made. The latter investigation will be based on the observation that the temperature dependence of the conduction electron shift in platinum metal is very large compared with other metals. This leads to the question whether there is an intrinsic temperature effect which influences the behavior of the electrons quite apart from their density. A basic change in the character of the wave functions could explain the observations of temperature dependence but the source of this basic change is not known.

The nuclear magnetic resonance of nickel in powdered nickel is being examined with available and marginal equipment, during the time that the permanent equipment for the project is being constructed. The nickel absorption has been observed and the work is being extended to alloys.

F. Anharmonic Effects in Solids - A. V. Granato

Anharmonic effects in solids will be studied using ultrasonic techniques. Information will be collected on the elastic constants together with the temperature and stress coefficients of the elastic constants of selected materials. The immediate objective of the program is the construction of apparatus necessary for measurements as a function of temperature, pressure and uniaxial stress. Long-range objectives include (1) the checking (with the help of accurate data to be obtained) of relations which can exist between various anharmonic effects; (2)the establishment of an equation of state of solids useful in the megabar range; (3) the determination of interatomic potentials and (5) the calculation of defect properties in crystals.

It has not been possible in the past to measure the five second order elastic constants of cubic crystals because the uniaxial stresses required lead to shear stresses which caused the crystal to deform plastically. It is proposed to overcome this difficulty by making two experimental improvements. First, by use of an ultrasonic interferometric technique, a great increase in sensitivity over previous measurements can be obtained. Secondly, the strength of crystals can be increased by irradiation. It is believed that a combination of these two improvements will make feasible the desired experiments.

III. Defect-Controlled Properties of Solids

A. Magnetic Resonance - C. P. Slichter

This project proposes to continue studies of magnetic resonance in solids concentrating on point imperfections using electron spin resonance. The structure of paramagnetic crystals, principally centers in the alkali halides involving an excess of electrons such as R and Z centers, will be investigated. The technique

of electron nuclear double resonance will be used which will permit the acquisition of much greater detail than electron spin resonance alone. Nuclear resonance in insulators and metal single crystals will be used to study lattice distortions and electron distributions about chemical impurities. In part, conventional single resonance techniques will be used but the nuclear double resonance method will also be used. Relatively little resonance work has been done on metal single crystals. It should be possible to study atoms near to impurities in metal single crystals since their resonance will not be smeared out by the angular average encountered in the usual part of the samples. On the basis of studies using impurities, it will be possible to decide whether or not studies of interstitials and vacancies are possible.

B. Point Imperfections in Solids - D. Lazarus

This program is concerned with experimental and theoretical investigations of point defects in solids, in particular, their relationship to diffusion processes. The experimental techniques employed involve precision sectioning methods using radioactive tracers and elastic relaxation methods, measurements of electrical resistivity, nuclear magnetic resonance (NMR) techniques and methods for generation of high hydrostatic pressures. Currently tracer investigations are being carried out to study self and impurity diffusion in transition metals as a function of temperature and pressure. Association of point defects with impurities, dislocations and other point defects is being studied by quenched resistivity and elastic relaxation and NMR methods. NMR techniques are also being employed to determine correlations effects in diffusion and to investigate diffusion in liquid metals. Tracer and optical techniques are employed in studies of the effect of electrical and thermal gradients on diffusion.

C. Point Defect - Dislocation Interactions - H. K. Birnbaum

Experimental and theoretical studies have been made of low temperature strain aging effects after deformation of copper and additional equipment for similar work on aluminum is being constructed.

Equipment for measurement of internal friction and elastic modulus in the frequency range from 1 cps to 100 kc and the temperature range from $4^{o}K$ to $273^{o}K$ is being constructed.

The yield stress and the work hardening rate of quenched polycrystalline gold is being examined. The results indicate that the quench hardening mechanism which affects the initial yielding differs from that which operates after a small deformation.

The purpose of this project is to investigate point defect-dislocation interactions and to examine the types of point defects formed during plastic deformation.

Strain aging experiments are performed on high purity aluminum and from the results of these experiments, the activation energies for point defect diffusion in the lattice and along dislocations is being measured.

The nature of the Bordoni peak damping mechanism is being investigated. The height of the maximum and peak temperatures of the Bordoni damping peaks will be measured after small plastic deformations at $4^{\circ}K$ and annealing in the range from $4^{\circ}K$ to $273^{\circ}K$.

Quench hardening experiments with gold and aluminum will be carried out. The detailed aging kinetics and the kinetics of resofting will be investigated. It is believed that there are two distinct types of interaction during aging after quenching. One type leads to an increase in yield stress and a small yield point; the other causes a change in the rate of work hardening.

Vacancies will be quenched into the lattice and the interaction of them with dislocations will be studied through measurements of internal friction and elastic modulus. Using gold foils, the amplitude dependence of the damping and temperature pulsing experiments will permit a measurement of the vacancy-dislocation binding energy.

D. Dislocation and Surface Barriers - M. Metzger

The effect of thin surface films on the strength of metal crystals will be investigated. Copper and zinc crystals will be used with adherent electroplated films and with organic coatings. The objective is to obtain evidence concerning the interaction between dislocations in the substrate crystal and the surface barrier and concerning the manner in which the dislocation structure of the substrate is altered to yield the observed hardening.

Another aspect of the interaction that will be studied is the relation between the manner in which the film accommodates slip in the substrate (cracking, shearing, or detachment), the properties of the film and the dislocation configuration in the substrate.

The techniques used will include tension tests and anelastic measurements. Surface structure will be studied by optical and electron microscopy. Dislocation etch pit studies will be a primary tool for studying metallic structure.

E. Annealing of Cold Worked Metals - B. G. Ricketts

This project is concerned with the fundamental structural changes which occur through deformation and annealing of metals, in particular those changes which can be observed advantageously by means of electron transmission microscopy.

The mechanism of nucleation of recrystallization as related to polygonization and subgrain growth is being investigated for cold rolled aluminum and copper. The annealing of stacking faults in cold rolled copper-base alloys is being investigated. As attempt is being made to estimate the stacking fault energy through observation of extended dislocation nodes. The mechanism for annealing out of stacking faults is being sought. The structure of the radiation damage in deuteron irradiated silver is being examined under the electron microscope. The effects of solutes on recovery processes in silver will also be sought.

F. Research on Radiation Damage - J. S. Koehler

This project aims to determine the nature and number of lattice imperfections introduced into crystalline solids by nuclear irradiation at liquid helium temperature. In addition, it would like to discover the nature of the various annealing processes which occur as the temperature of the specimen is increased. The activation energy or spectrum of activation energies associated with the motion of each particular lattice defect also constitutes a portion of the desired information. The project also aims to determine the nature and magntude of the changes in physical properties which result from a given concentration of a particular kind of lattice defect. The defects which are believed to be of importance are interstitial atoms, lattice vacancies, crowdions, small inclusions of another solid phase and possible precipitates of interstitial atoms. The properties investigated are resistivity, volume, lattice parameter and stored energy. The crystals examined are copper, silver, gold, iron, nickel, cobalt, GaSb, InSb, germanium, silicon and various alloys.

Specific subjects under study are: (1) small angle x-ray scattering by defects; (2) Schottky defects in AgCl; (3) the nature of Stage III annealing in Cu, Ag, and Au; (4) production of interstitials by ion bombardment of foils; (5) attempt to determine atomic configuration around an interstitial by x-ray scattering; (6) theoretical calculations of defect properties in Ge and Si; (7) study of irradiation effects in Ge foils; and (8) deformation and vacancy annealing in gold.

IV. Phase Changes and Precipitation in Alloys and Glasses

A. Diffusionless Phase Changes in Non-Ferrous Metals and Alloys
T. A. Read

The purpose of the work is to conduct studies of quenched-in defects and transformation behavior in beta phase alloys. The annealing behavior of quenched alloys is followed by resistivity measurements and thin film electron microscopy. The transformation behavior is studied with regard to nucleation, growth, and internal structure of the product phase. This will also be done by transmission electron microscopy.

Other phases of the work include studies of transformation kinetics by means of oscillographic recording of electrical resistivity changes. More quantitative information will be obtained on the point defect content of quenched beta phase alloys through combined lattice parameter and density measurements.

B. Enthalpy Changes in Athermal Solid State Transformations
C. J. Altstetter

The purpose of this project is to obtain reliable values for the enthalpy changes that occur during martensitic transformations. Such data are needed for the thermodynamic analysis of these transformations.

An accurate calorimeter is to be constructed that will require no machining of the specimen because of the brittle nature of some of the materials to be examined. The displacive nature of martensitic transformations makes it desirable to eliminate mechanical constraints which would tend to cause or prevent transformation.

The proposed calorimeter will maintain a constant temperature difference between the specimen and its enclosure. The value of the transformation enthalpy change will be obtained from the magnitude of the anomaly in the heating or cooling curve.

Initially a material such as Au-49% Cd or Fe-30% Ni having a transformation near room temperature will be examined but the calorimeter will be designed for higher temperatures so that annealing can be carried out in it.

C. Structural Changes in Simple Glass Systems During Nucleation of Crystalline Phases - C. G. Bergeron

The identification and analysis of structural changes which occur in simple inorganic oxide glasses as a function of temperature and time is the subject of this project. As in previous work of this project, the glass systems are of the silicate and borate types with and without titania additions.

Samples of these glasses will be heat treated in air at temperatures that have been partially defined by differential thermal analysis, viscosity, and resistivity measurements. The structural changes in the heat treated glasses will be investigated by x-ray scattering and the electron microscope will be employed to detect evidence of glass separation, nuclei formation, and crystal growth.

D. Structural Changes in Simple Glass Systems During Nucleation of Crystal Phases - A. L. Friedberg

This project is a study of the structural changes which precede the nucleation of crystalline phases in glasses. Lead borate and lead silicate glasses are the systems studied.

The rates of crystal growth of lead titanate from lead borate and lead silicate glasses have been determined. Shear viscosity and electrical conductivity have been investigated as a function of temperature as has the change in electrical conductivity with time for temperatures within the crystal growth range.

Optical and electron microscopy have been used to study microstructural changes during crystal growth. Thermal effects associated with structural changes occurring during nucleation, growth, and solution of the crystalline phase have been studied. The effect of an electric field during crystallization has been the object of preliminary study.

Particulate glass systems have been studied in the past with regard to their usefulness as ceramic coatings and, more recently, as ceramic structures. These systems are formed, mainly, by sintering or coalescence of particles. Investigation of the glass sintering phenomenon has shown that transport of matter takes place

chiefly through viscous glow. Grain boundaries in particulate glass systems appear similar in behavior to those of crystalline sintered systems.

In future work, the sintering phenomenon in particulate glass systems will be studied with emphasis on not only the sintering kinetics but also on other characteristics of these systems, such as gas solubility and crystallization behavior, that are associated with the large specific surface.

The initial program, exploratory in nature, will concentrate on (1) the kinetics of grain boundary formation and disappearance, (2) techniques for delineating the interfacial surfaces of grain boundary material and (3) the effect of environment on the sintering kinetics.

Recent Publications:

H. G. Drickamer and A. S. Balchan, "High Pressure Optical and Electrical Measurements," Modern Very High Pressure Techniques, Ed. R. H. Wentorf, Butterworth's London (1962 pp. 25-50.

H. G. Drickamer and S. Minomura, "Pressure Induced Phase Transitions in Silicon, Germanium, and some III-V Compounds," J. Phys. Chem. Solids 23, (1962) pp. 451-456.

H. G. Drickamer and G. A. Samara, "Pressure Induced Phase Transitions in Some II-VI Compounds," J. Phys. Chem. Solids 23, (1962) pp. 457-463.

H. G. Drickamer and G. A. Samara, "The Effect of Pressure on the Resistance of Three Thallous Halides," J. Chem. Phys. 37, (1962) pp. 408-410.

H. G. Drickamer and G. A. Samara, "The Effect of Pressure on the Resistance of Pyrolytic Graphite," J. Chem. Phys. 37, (1962) pp. 471-474.

H. G. Drickamer and G. A. Samara, "The Effect of Pressure on the Resistance of Fused Ring Aromatic Compounds," J. Chem. Phys. 37, (1962) pp. 474-479.

R. O. Simmons, J. S. Koehler, and R. W. Balluffi, "Present Knowledge of Point Defects in Irradiated Face-Centered Cubic Metals," IAEA Symposium on Radiation Damage in Solids and Reactor Materials (Venice, Italy, May 1962) Vol. I, p. 155.

Contractor:	Illinois Institute of Technology, Chicago, Illinois
Contract Number:	AT(11-1)-1052
Present Contract Term:	June 15, 1962 through June 14, 1963
Cost to AEC:	$18,555
Contract Title:	INVESTIGATION OF ENERGY TRANSFER PROCESSES BY FLASH PHOTOLYSIS
Investigators:	Leonard I. Grossweiner

Scope of Work:

Mechanisms of energy transfer in condensed substances are studied with pulse irradiation methods:

1. An investigation of low-temperature optical bleaching of color centers in KCl shows that illumination establishes an equilibrium between F and F' centers. The equilibrium constant is not sensitive to the method of coloration or the light intensity, showing that equilibrium occurs within local regions of the crystal. The results are explained by a mechanism involving the photoionization of F and F' centers and electron capture by F centers and negative-ion vacancies. The application of the model leads to 0.020 ± 0.003 for the photoionization efficiency of the F center at 80° K and 0.016 ± 0.005 for the ratio of the electron-capture cross section of the F center to the chloride-ion vacancy.

2. The sensitization of the photoconductivity of zinc oxide thin layers by adsorbed organic dye is under investigation. Eosin sensitizes the photoconduction of zinc oxide to green light. The kinetics indicate that a two-step mechanism takes place: excitation with a fast second-order decay in the dye, followed by energy transfer and a first-order production and decay of carriers in zinc oxide.

3. The detailed mechanism for the photosensitized oxidation of aqueous phenol by eosin dye has been determined and the reaction velocity-constants for the elementary processes have been measured. The predominant steps are the oxidation of phenol by triplet-state eosin and a back-reaction of the phenoxy radical with the semi-reduced eosin radical. A kinetic method for measuring the dissociation constant of short-lived free radicals has been developed and applied.

Recent Publications:

L. E. Silverman and L. I. Grossweiner, "Bleaching and Recovery of F Centers in KCl," Phys. Rev. 121, (1961) pp. 1072-75.

L. I. Grossweiner and E. F. Zwicker, "Transient Measurements of Photochemical Processes in Dyes.I. The Photosensitized Oxidation of Phenol by Eosin and Related Dyes," J. Chem. Phys. 34, (1961) pp. 1411-17.

A. R. Reinberg and L. I. Grossweiner, "Low-Temperature Optical Bleaching of F Centers in KCl," Phys. Rev. 122, (1961), pp. 1734-41.

A. Costikas and L. I. Grossweiner, "The Photoequilibrium Between F and F' Centers in KCl at 80°K," Phys. Rev. (in print)

Contractor: IBM Corporation, Yorktown Heights, New York

Contract Number: AT(30-1)-2811

Present Contract Term: May 15, 1962 through May 14, 1963

Cost to AEC: $56,232

Contract Title: DEFECTS IN METALLIC AND IONIC CRYSTALS

Investigators: Arthur S. Nowick

Scope of Work:

Point defects are being studied in metals and alkali halides by techniques which tend to differentiate between the various types. Primary attention is being given to relaxation processes, both anelastic and dielectric. Anelastic relaxation occurs when the elastic distortion about the defects locally lowers the stress then produces time dependent deformation of the crystal due to reorientation of these "elastic dipoles" into preferential positions created by the applied stress. In an analogous way one may obtain dielectric relaxation of an insulator in an electric field.

Among the defects being studied by anelasticity are the solute-solute pair (the Zener relaxation effect) and the solute-vacancy pair. Also, the change of electrical resistance accompanying the Zener relaxation ("anelastic Piezoresistance") is being studied. Finally the Zener effect is being used to observe the kinetics of vacancy formation and annealing in solid solutions.

Dielectric relaxation is being studied in alkali halides for dipoles consisting of the divalent cation impurity associated with a cation vacancy. Electrical measurements in the alkali halides also measure the steady d.c. conductivity of vacancies unassociated with impurities at each temperature.

Recent Publications:

R. W. Dreyfus and A. S. Nowick, "Energy and Entropy of Formation and Motion in Vacancies in NaCl and KCl Crystals," J. Appl. Phys. 33, (1962) p. 473

A. S. Nowick and B. S. Berry, "The Zener Relaxation as a Distribution of Relaxation Times," Acta Met., 10 (1962) p. 312.

B. S. Berry, "Review of Internal Friction due to Point Defects," Acta Met, 10, (1962) p. 224.

Contractor: Johns Hopkins University, Baltimore, Maryland

Contract Number: AT(30-1)-2185

Present Contract Term: June 1, 1962 through May 31, 1963

Cost to AEC: $35, 125

Contract Title: REDETERMINATION OF ABSOLUTE X-RAY WAVELENGTH STANDARD

Investigators: J. A. Bearden

Scope of Work:

Measurements for the establishment of the Angstrom as a standard for x-ray wavelengths in crystal dimensions are being made. The interpretation of recent x-ray and density measurements on silicon crystals, as well as the precision measurement on the gamma ray annihilation radiation wavelengths now depends on the absolute scale of x-ray wavelengths. The fundamental constants α and Avogadro's number N are intimately involved in the interpretation which depends on the ruled grating measurements.

Successful measurements of the high frequency limit of the continuous x-ray spectrum with a gas target x-ray tube open a new field of x-ray spectroscopy. New measurements on excitation properties, fluorescent excitation, polarization, distortion of spectra and spectral intensity as a function of energy are proposed.

The importance of small variations in lattice parameters of polycrystalline materials has resulted in a series of papers on the relative merits of the "centroid" vs. "peak" method of measuring the diffracted x-ray spectral lines. A new precision study of the spectral line profile for the $K\alpha_1 \alpha_2$ lines of copper and iron is proposed, in which good calcite, quartz, and silicon crystals will be employed. The percent deflection measured, the effect of voltage (DC and AC) evaluated, effect of path absorption and nickel absorbers measured, and the importance of x-rays diffracted by "tails" of the x-ray window examined.

Contractor: Johns Hopkins University, Baltimore, Maryland

Contract Number: AT(30-1)-2543

Present Contract Term: May 1, 1962 through April 30, 1963

Cost to AEC: No-Fund Extension

Contract Title: PRECISION X-RAY WAVELENGTHS

Investigators: J. A. Bearden

Scope of Work:

A precise conversion of the Siegbahn X-unit scale of x-ray wavelengths to Angstroms has been the aim of a number of extensive ruled grating research programs for the past thirty years. Regardless of the success of such measurements, the extensive wavelength measurements reported in x-ray literature cannot be accurately corrected to the new absolute scale by the use of a simple multiplying factor. The research program aims to remeasure with calibrated crystals a few x-ray lines used in each of the best reported experimental programs, in order to correct the published values to both a consistent and absolute scale. In addition, the wavelengths and energies of the absorption spectra of the different authors can be recalculated with the aid of the redetermined emission lines which were used in the original researches for calibration. This will remove from the literature much of the confusion which now exists in the values reported by various authors.

The research program will make use of the precision double crystal spectrometer with quartz and silicon crystals whose grating constants have been measured in terms of the standard meter to remeasure selected emission lines from each of the best published researches. It will be necessary to remeasure some 200 to 300 x-ray lines from some 3000 published values in order to establish a proper correlation of the wavelengths from 0.1 A to 10.0 A. The principal technical problems involved arise in the construction of appropriate x-ray sources, detectors, and in measurements of the actual wavelengths over the energy range of 1 to 100 kev. In addition, there are the problems of developing appropriate recording techniques and the application of appropriate correction factors which are required to make the results definitive and unambigous.

Contractor: Kansas, University of, Lawrence, Kansas

Contract Number: AT(11-1)-1197

Present Contract Term: June 1, 1962 through May 31, 1963

Cost to AEC: $50,220

Contract Title: POINT DEFECTS IN IONIC CRYSTALS

Investigators: Robert J. Friauf

Scope of Work:

Investigations are to be made of both ionic and electronic defects. Ionic defects are studied by means of correlation effects in diffusion; measurements of ionic conductivity play an important supporting role. Proposed experiments are: (1) Continuation of work in progress for diffusion of Tl and Cl in TlCl. (2) Initiation of diffusion measurements with an applied electric field in an attempt to detect a possible contribution of vacancy pairs to diffusion in TlCl and perhaps in NaCl. (3) Accurate determination of diffusion of Ag in AgCl to allow evaluation of interstitialcy migration energies.

Electronic defects in the form of color centers are to be studied by measurements of optical absorption, polarized bleaching and luminescence, and electron and double resonance. Particular attention is directed to Z centers in KCl and perhaps NaCl and LiF. Proposed experiments are: (1) An attempt to produce Z centers in LiF with Mg. (2) Polarized bleaching and luminescence measurements for Z centers in KCl, NaCl, and perhaps LiF. (3) Double resonance experiments on Z centers in KCl with isotopically enriched Sr^{87} or Ba^{137}.

Theoretical calculations needed for the interpretation of experimental results are contemplated in connection with (1) correlation effects in diffusion and (2) wave functions of electrons at F and Z centers.

Contractor: Little, Arthur D., Inc., Cambridge, Massachusetts

Contract Number: AT(30-1)-2756

Present Contract Term: April 15, 1962 through April 14, 1963

Cost to AEC: $42,200

Contract Title: ROLE OF LATTICE IMPERFECTIONS IN BEHAVIOR OF SOLIDS

Investigators: Richard S. Davis

Scope of Work:

I. Interaction of defects with surfaces.

This research project is directed toward an improved understanding of the interaction of vacancies with surfaces in aluminum. It has been shown that during cooling from elevated temperatures, vacancies condense at the surfaces of electropolished aluminum single crystals to form pits. A study is being conducted in which the supersaturation necessary to nucleate pits is measured as a function of temperature and surface orientation. The results will be analyzed on the basis of nucleation theory. In particular, it will allow us to measure the temperature dependence of a nucleation process and compare the results with theoretical predictions.

II. Oxidation of Aluminum.

For the past year, work has been in progress related to a direct observation of the oxidation of high purity aluminum single crystals utilizing a new experimental technique. This has led to the identification of a two-stage process; a low temperature (below 500°C) amorphous oxide which grows by the transport of cations, and a high temperature (above 500°) crystalline oxide which grows by the transport of anions. This work is being continued, and shall be extended to aluminum alloy systems.

Recent Publications:

P. E. Doherty, R. S. Davis, "Observations of the Structure of Aluminum Specimens Grown from the Melt," Trans. Met. Soc., AIME, Vol. 221, No. 4, (1961) pp. 737-740.

P. E. Doherty, R. S. Davis, "The Formation of Surface Pits by the Condensation of Vacancies," Acta Met. Vol. 7, (1959)

Contractor: Louisiana State University, Baton Rouge, Louisiana

Contract Number: AT(40-1)-3087

Present Contract Term: February 15, 1963 through February 14, 1964

Cost to AEC: $45,903

Contract Title: CONDUCTIVITY TENSORS IN METALS AND SEMICONDUCTORS

Investigators: J. M. Reynolds

Scope of Work:

The electrical magnetoresistance, the Hall effect, the thermal magnetoresistance, the Righi-Leduc effect, the thermoelectric effect, the Ettingshausen-Nernst effect, the Peltier effect and the Ettingshausen effect will be accurately measured in single crystals of several metals and semiconductors. These measurements will be made for various crystallographic orientations at temperatures thoughout the liquid helium range (also at liquid hydrogen temperatures when needed) and in magnetic fields from zero up to 60 kilogauss. The data obtained will be used to construct the complete electrical, thermal, and thermoelectric tensors for each material. From these tensors the conductivity tensor elements (kinetic coefficients) will be calculated and compared with those computed from transport theory. Among the metals to be studied are magnesium, cadmium, tin, antimony, and bismuth. Measurements are also planned on indium antimonide, and indium arsenide.

Contractor: Maryland, University of, College Park, Maryland

Contract Number: AT(40-1)-2068

Present Contract Term: March 15, 1962 through March 14, 1963

Cost to AEC: $15,329

Contract Title: PROCESSES OF DIFFUSION AND ELECTRICAL CONDUCTION IN SOLIDS

Investigators: Homer W. Schamp, Jr.

Scope of Work:

This program is concerned with determining the pressure and temperature dependence of diffusion and electrical conductivity in alkali halides. Measurement of diffusion of the chloride ion in sodium chloride and potassium chloride at high pressure are under way and a method of measuring electrical conductivity of the alkali halides at high pressures in the solid cell is being developed.

Contractor: Massachusetts Institute of Technology, Cambridge, Mass.

Contract Number: AT(30-1)-1002, Scope I

Present Contract Term: September 1, 1962 through August 31, 1963

Cost to AEC: $51,300

Contract Title: THERMODYNAMICS AND OTHER ASPECTS OF METALLIC SYSTEMS

Investigators: M. B. Bever

Scope of Work:

In this study of the thermodynamic properties of metallic systems recent emphasis has been on the influence of crystalline imperfections on thermodynamic properties. This has involved measurements of stored energy and annealing kinetics of metals and alloys using speed of prior deformation, temperature of deformation, and degree of order as variables. In relation to the work on effects of speed of deformation, a comparison has been made of the effects of explosive loading on stored energy and annealing kinetics to the effects of loading at more conventional speeds; significant difference in behavior has been observed.

Recent Publications:

J. B. Cohen, B. W. Howlett and M. B. Bever, "The Heats of Solution in Liquid Tin of the Group III Elements Aluminum, Gallium, Indium and Thallium," Trans. Met. Soc. of AIME, Vol. 221, (1961) pp. 683-686.

B. Roessler and M. B. Bever, "The Effects of Deformation at 78°K on the Alloy Cu_3Au," Trans. Met. Soc. of AIME, Vol. 221, (1961) pp. 1049-1055.

B. W. Howlett, J. S. L. Leach, L. B. Ticknor and M. B. Bever, "Liquid Metal Solution Calorimeter," Review of Scientific Instruments, Vol. 33, (1962) pp. 619-624.

G. Scatchard and T. P. Lin, "The Equilibrium of alpha-Silver-Zinc-Cadmium Alloys with Zinc and Cadmium Vapors," J. of American Chem. Soc., Vol. 84, (1962) pp. 28-84.

Contractor: Massachusetts Institute of Technology, Cambridge, Mass.

Contract Number: AT(30-1)-1310

Present Contract Term: October 15, 1962 through October 14, 1963

Cost to AEC: $21,150

Contract Title: MECHANICAL PROPERTIES OF METALS AT LOW TEMPERATURES

Investigators: W. A. Backofen

Scope of Work:

The deformation characteristics of copper single crystals with [011], [001], and [111] multiple-slip orientations are being studied at low temperatures. To date most of the tension tests have been made at 4.2 and 78°K. Mechanical twinning was observed in [111] crystals, initiating during stage II hardening (τ = 26,000 psi) at 4.2°K and during stage III hardening (τ = 34,000 psi) at 78°K. Compression tests of [001] crystals are planned to determine whether a critical resolved shear-stress low exists for twinning.

For the orientations tested, the fact of equal stress on four or more slip systems did not always result in the same extent of operation by these systems throughout the deforming crystal. Inhomogeneous deformation was observed in all [011] crystals and in some of the [001] crystals. In the latter case, the work hardening rate was lower but more nearly linear when deformation was inhomogeneous. The reasons for such differences in deformation behavior are being studied. The deformation of [111] crystals was comparatively homogeneous with slip along the three favored directions throughout.

Further testing of multiple-slip single crystals and polycrystalline specimens is to be carried out at other temperatures and under conditions of abrupt temperature change.

A related investigation has been made of the ductile fracture problem using high purity aluminum as test material. The results have made it possible to evaluate contributions of adiabatic shear and void nucleation to the over-all fracture process. In particular, there is no evidence of either vacancy condensation or dislocation cracking in fracture nucleation. Below about 40°K, there is good evidence of grainboundary sliding and cracking in the polycrystalline material.

Contractor:	Massachusetts Institute of Technology, Cambridge, Mass.
Contract Number:	AT(30-1)-1985
Present Contract Term:	March 1, 1962 through February 28, 1963
Cost to AEC:	$27,747
Contract Title:	KINETICS OF REACTIONS BETWEEN LIQUID METALS AND LIQUID SALTS
Investigators:	Thomas B. King

Scope of Work:

The rate and mechanism of reactions between liquid alloys and liquid salts are being studied by direct and electrochemical methods.

It has been established that, for most reactions involving halide salts, transport control of the rate is to be expected. Control is usually by the transport of a solute in the alloy phase, particularly where low concentrations are involved and where the free energy change for the reaction is high. Mixed control, involving the contribution of transport in the salt phase has also been demonstrated. Model experiments, at low temperatures have revealed the quantitative dependence of the rate of such reactions on system geometry and convection conditions.

Direct rate experiments on the reduction of silica, dissolved in a silicate, by aluminum, dissolved in a copper alloy, have shown that the likely rate-controlling process is transport of silica in the silicate phase. If this is so, the diffusion coefficient of silicon in the salt phase is strongly influenced by the composition of the silicate.

Electrochemical studies of the evolution of CO at a carbon electrode in an oxide (silicate) melt suggest that the major part of the anode overpotential is activation overpotential. The results are compatible with control of the rate of the electrode reaction by the discharge of an oxygen ion.

Attention is being concentrated on electrochemical techniques; reactions at a silicon electrode in a silicate melt are now being studied. This system is chosen, since it is known that the electrode process involves a relatively high activation energy, and it is presumed that the electrode reactions, in contradistinction to those occurring in halide melts, are not very fast.

Measurements of diffusion coefficients in certain liquid alloys are being continued; such data are necessary for satisfactory interpretation of rate measurements.

Contractor: Massachusetts Institute of Technology, Cambridge, Mass.

Contract Number: AT(30-1)-2574

Present Contract Term: September 1, 1962 through August 31, 1963

Cost to AEC: $200,150

Contract Title: SOLID-STATE STUDIES IN NON-CRYSTALLINE SYSTEMS

Investigators: W. D. Kingery

Scope of Work:

The purpose of this program is to investigate: (a) the effect of forming processes and kinetic phenomena on microstructure development in ceramics and short-range order structures and (b) the relationship of physical properties to crystal structure, microstructure, and the structure of non-crystalline solids.

Forming processes being investigated include compaction processes, vapor deposition of non-crystalline solids, and crystal growth from the vapor phase at elevated temperature. Studies of compaction processes are concentrated on understanding the formation of green ware in a qualitative way; vapor deposition processes include deposition of Al_2O_3 and other oxides. Vapor phase deposition on a cold substrate to form a structure having no long-range order is also being investigated; structural analysis of the resulting product is being carried out by micrographic and x-ray analysis together with optical spectroscopy of samples containing small amounts of transition elements. Crystal deposits from vapor phases are being investigated to quantitatively determine the vapor pressure conditions necessary and its relationship to the morphology of the product formed.

Mechanical property studies include the properties of glasses at elevated temperatures and high strain rates, and deformation of polycrystalline oxides with particular regard to boundary deformation processes. Electrical phenomena in glasses include properties, glasses formed outside the normal melting range by vapor deposition, and investigation of semiconducting characteristics of glasses heat-treated at high and low oxygen pressures.

Recent Publications:

A. R. Cooper, Jr., and W. H. Goodnow, "The Examination of Density Distributions in Dry Pressed Compacts of Ceramic Powders by Radiography of Lead Grids," Bull. Am. Ceram. Soc., in press.

A. R. Cooper, Jr. and L. E. Eaton, "Compaction Behavior of Several Ceramic Powders," J. Am. Ceram. Soc., in press.

P. J. Koros and T. B. King, "Diffusion of Oxygen in a Lime-Alumina-Silica Slag," Trans. AIME, in press.

A. R. Cooper, Jr. and W. D. Kingery, "Kinetics of Solution in High Viscosity Liquids: Sodium Chloride-Glycerine," J. Phys. Chem., in press.

A. R. Cooper, Jr. "The Effect of the Moving Boundary on Unsteady State Diffusion Controlled Dissolution or Growth of Slabs," Trans. Faraday Soc., in press.

A. R. Cooper, Jr., "Dissolution Kinetics in Glass-Making," VI International Congress on Glass, in press.

W. D. Kingery and G. E. Meiling, "Transference Number Measurements for Aluminum Oxide," J. Appl. Phys., 33, (1961) p. 556.

W. D. Kingery, E. Niki, and M. D. Narasimhan, "Sintering of Oxide and Carbide-Metal Compositions in the Presence of a Liquid Phase," J. Am. Ceram. Soc., 44, (1961) p. 29.

R. L. Coble with J. E. Burke, "Review of Sintering in Ceramics," to appear in PROGRESS IN CERAMIC SCIENCE, J. E. Burke, Editor (Volume 3)

W. D. Kingery, "Heat-Conductivity Processes in Glass," J. Am. Ceram. Soc., 44, (1961) p. 302.

J. Pappis and W. D. Kingery, "Electrical Properties of Single-Crystal and Polycrystalline Alumina at High Temperatures," J. Am. Ceram. Soc., 44, (1961) p. 459.

W. D. Kingery, "The Thermal Conductivity of Ceramic Dielectrics," PROGRESS IN CERAMIC SCIENCE, Vol. 2, J. E. Burke, Editor (1962)

A. S. Michaels and R. G. Miekka, "Polycation-Polyanion Complexes: Preparation and Properties of Poly-(Vinylbenzyltrimethylammonium) Poly-(Styrenesulfonate), J. Phys. Chem., 65, (1961) p. 1765.

R. S. Feigelson and W. D. Kingery, "Physical Properties of Polycrystalline Silicon Borides," Submitted for publication, J. Am. Ceram. Soc.

W. D. Kingery, J. M. Woulbroun, and F. R. Charvat, "Effect of Applied Pressure on Densification during Sintering in the Presence of a Liquid Phase," Submitted for publication, J. Am. Ceram. Soc.

Contractor: Massachusetts Institute of Technology, Cambridge, Mass.

Contract Number: AT(30-1)-2879

Present Contract Term: September 1, 1962 through August 31, 1963

Cost to AEC: $120,205

Contract Title: ATOMIC ARRANGEMENTS AND IMPERFECTIONS

Investigators: B. L. Averbach and Morris Cohen

Scope of Work:

Atomic arrangements and imperfections are being investigated in a variety of materials. The atomic arrangements are being studied by means of diffuse x-ray scattering measurements and the imperfections by means of transmission electron microscopy and etch-pit techniques. A high speed digital computer is being used to evaluate the x-ray data and to make theoretical calculations of solid solution models. Research is underway on the study of the thermodynamic properties and the short-range order in iron-silicon alloys and on the nucleation of the precipitation products in the gold-nickel alloys. The use of electron diffraction techniques for the study of imperfections is also being investigated.

The influence of imperfections on the self-diffusion coefficient is being investigated in gold. The specimen is arranged to be in compression creep during the diffusion anneal, and preliminary results indicate that the self-diffusion coefficient can be increased by a factor of about 10^5 under these conditions.

Recent Publications:

S. V. Radcliffe, B. L. Averbach and Morris Cohen, "Relative Thermodynamic Properties of Solid Iron-Aluminum Alloys," Acta Met. 9, (March 1961) p. 169.

J. M. Dupouy and B. L. Averbach, "Atomic Arrangements in Titanium-Molybdenum Solid Solutions," To be published in Acta Met.

M. Hillert, "A Solid Solution Model for Inhomogeneous Systems," To be published in Acta Met.

M. Hillert, M. Cohen, and B. L. Averbach, "Formation of Modulated Structures in Copper-Nickel-Iron Alloys," To be published in Acta Met.

G. Nagorsen and B. L. Averbach, "Small-Angle Scattering in Gold-Nickel Alloys," J. of Applied Physics, 32, (1961) p. 688.

Recent Publications:

M. J. Hordon and B. L. Averbach, "X-Ray Measurements of Dislocation Density in Deformed Copper and Aluminum Single Crystals," Acta Met. 9, (1961) p. 237.

M. J. Hordon and B. L. Averbach, "Precision Density Measurements on Deformed Copper and Aluminum Single Crystals," Acta Met. 9, (1961) p. 247.

Contractor: Massachusetts Institute of Technology, Cambridge, Mass.

Contract Number: AT(30-1)-2909

Present Contract Term: February 1, 1963 through January 31, 1964

Cost to AEC: $13,500

Contract Title: EFFECT OF RADIATION ON CRYSTAL GROWTH RATES

Investigators: Edward A. Mason and Robert C. Reid

Scope of Work:

Atomic displacements result from irradiation of crystals. If suitable irradiation is used while the crystal is growing from a solution, it is reasonable to predict that such displacements will affect the rate of growth. Even in cases where no appreciable atomic displacements result, there is a good possibility that other radiation-induced surface effects (such as ionization, temperature spikes, etc.) will affect the rate of two-dimensional nucleation.

At present we are studying the growth of freely suspended seed crystals of succinic acid under conditions of constant temperature and supersaturation. Growth experiments are carried out first without irradiation and the results will be compared with similar tests using a Co^{60} irradiation source. Equipment fabrication is nearing completion and initial irradiations will be made in 1963.

Contractor: Massachusetts Institute of Technology, Cambridge, Mass.

Contract Number: AT(30-1)-3020

Present Contract Term: June 1, 1962 through May 31, 1963

Cost to AEC: $12,500

Contract Title: A STUDY OF RADIATION DAMAGE

Investigators: B. E. Warren

Scope of Work:

This study showed that in the severe cold working which is present in filings, the stacking faults extend completely across the coherent domains rather than being confined to rather narrow ribbons as commonly pictured. It is important to emphasize that this result has been established only for the case of severe cold working in bulk materials. Additional information about the nature of cold work distortion in metals is being obtained by the use of alloys originally in a long range ordered state. Studies using ordered Cu_3Au have continued through the year.

In the coming year it is hoped to finish the work using ordered Cu_3Au. BCC metals are the ones for which one gets the least information about the cold worked state from an x-ray examination. It is hoped to get more detailed information for the BCC materials by the use of a sample in which preferred orientation has been introduced by the cold work, and also by the use of BCC alloys initially in a long range ordered state. It is also hoped to study the practical applications of the method for grain size measurement reported in NYO-4836.

Recent Publications:

B. E. Warren, "X-Ray Measurement of Stacking Fault Widths in FCC Metals," J. of Appl. Phys. Vol. 11, (1961) pp. 2428-2431. (Technical Rpt. NYO-4836)

B. E. Warren, "The Anomalous Temperature Behavior of the 200 Reflection of Fluorite," Acta Crystallographica, Vol. 14, Part 10, (1961).

Contractor:	Massachusetts Institute of Technology, Cambridge, Mass.
Contract Number:	AT(30-1)-3031
Present Contract Term:	June 1, 1962 through May 31, 1963
Cost to AEC:	$49,850
Contract Title:	NEUTRON DIFFRACTION STUDIES OF LOW TEMPERATURE PARAMAGNETIC ALIGNMENT IN SOLIDS
Investigators:	C. G. Shull

Scope of Work:

Polarized neutron radiation from the MIT Research Reactor is being used in studies of low temperature paramagnetic alignment as a means of determining the magnetic characteristics of paramagnetic atoms and ions. Information on both the spatial and directional configuration of the outer-atom magnetic electrons can be obtained from measurements of the scattering form factor. Single crystals of magnetic salts or metals are being subjected to high magnetic fields at liquid helium (and lower) temperature and the resulting coherent magnetic scattering is being examined. Experiments with vanadium crystals has shown electronic polarization scattering characteristic of 3d shell electrons rather than the expected 4s conduction electrons. Nuclear polarization scattering has also been measured in vanadium at temperatures below about 15°K. Other transition elements and paramagnetic atoms are being investigated.

Contractor:	Massachusetts Institute of Technology, Cambridge, Massachusetts
Contract Number:	AT(30-1)-3134
Present Contract Term:	November 1, 1962 through October 31, 1963
Cost to AEC:	$79,000
Contract Title:	FUNDAMENTALS OF DIFFUSION
Investigators:	R. E. Ogilvie

Scope of Work:

Three specific problems are being attacked, all by use of the microprobe analyzer. In the first, diffusion in the Cu/Ag/Au system will be studied and the results analyzed in terms of irreversible thermodynamics. The analog computor will be used to analyze the composition profiles of the diffusion couples in order to determine the variation in the cross terms in the Onsager relations as a function of composition.

The second problem involves measurement of solute diffusion in the neighborhood of a pure tilt boundary in silver bicrystals. One of the main objectives is to determine if the diffusion coefficients are concentration dependent, as would be expected if the dislocation wall in the boundary could be saturated. Another is to determine the directional dependence of diffusion coefficients near the wall. A treatment of the case for grain boundary diffusion with concentration-dependent diffusion coefficients has been worked out by one of Ogilvie's group and will be applied to the system studied.

In the third study to be conducted under this program, the microprobe will be applied to analysis of constituent distribution during oxidation of a binary alloy in which only one constituent participates in the oxidation process. The Ni-Pt system has been chosen for this. It is planned to measure the concentration profile in Ni, in the metal, and in the oxide as a function of oxidizing time and use the data to test current alloy oxidation theory.

Contractor: Massachusetts Institute of Technology, Cambridge, Mass.

Contract Number: AT(30-1)-3208

Present Contract Term: May 15, 1963 through May 14, 1964

Cost to AEC: $30,000

Contract Title: STUDIES ON THE DISTRIBUTION OF IMPURITIES IN SOLIDS

Investigators: Harry C. Gatos

Scope of Work:

The objective of this investigation is to further our understanding of the way impurities are distributed during the growth of a crystal from liquid. Part of the investigation will be devoted to further study of the growth of crystals in which the distribution of impurities has been observed to vary periodically.* The extent of supercooling at the solid liquid interface will be measured and its variations studied as a function of thermal gradient, impurity concentration and species.

Also, an attempt will be made to reveal and study the segregation of impurities to defects and the chemical behavior of defects (i.e. etch pitting at dislocations) as influenced by impurities.

*H. C. Gatos et.al., J. Appl. Phys. 32, (1961) p. 2057.

Contractor: Massachusetts Institute of Technology, Cambridge, Mass.

Contract Number: AT(30-1)-3168

Present Contract Term: February 14, 1963 through November 13, 1963

Cost to AEC: $27,240

Contract Title: IRRADIATION EFFECTS ON SURFACE REACTIONS

Investigators: M. T. Simnad and H. H. Uhlig

Scope of Work:

The oxidation kinetics of metals forming a protective oxide film is dependent on transport properties through the film. It is expected that the crystal imperfections introduced into such an oxide film by nuclear radiation will influence the reaction kinetics. In an investigation at General Atomics, Simnad has found that between 150 and 250°C, radiation does increase oxidation rate; above this range no effect is seen. These studies are being continued using the MIT reactor.

Contractor: Massachusetts Institute of Technology, Cambridge, Mass.

Contract Number:

Present Contract Term:

Cost to AEC: $40,000

Contract Title: RELATION OF STRUCTURAL DEFECTS AND MICROSTRUCTURE TO SUPERCONDUCTIVITY

Investigators: George W. Pearsall

Scope of Work:

Superconducting properties are subject to variations in thermal and deformation history, indicating that they depend on such characteristics of the material as the types and arrangements of defects present and the details of the microstructure. This program is to study the nature of this type of dependence in specific materials -- superconductors in which we already know that the structure can be changed in definite ways by altering the processing conditions. Initially, Nb_3Sn and other beta-W compounds are being used for the investigation of how defects influence superconductivity and Pb-Sn alloys will be used, starting with the eutectic, to investigate the importance of phase configurations in a two phase microstructure. The study of microstructural effects in a simple alloy system is intended to circumvent some of the difficulties associated with interpreting microstructures in more complex systems like Nb-Sn and Nb-Zr.

Contractor:	Massachusetts, University of, Amherst, Massachusetts
Contract Number:	AT(30-1)-3003
Present Contract Term:	May 1, 1962 through April 30, 1963
Cost to AEC:	$12,480
Contract Title:	STUDIES OF CRYSTAL ORIENTATION IN IRRADIATED CRYSTALLINE POLYMERS
Investigators:	Richard S. Stein

Scope of Work:

Films of polyethylene, polypropylene and/or poly-i-butene are prepared and crosslinked by radiation. The following types of studies are being made on these films:

(1) X-ray measurements on orientation of crystals grown from these oriented, melted films as a function of degree of orientation, temperature of melt and temperature of crystallization.
(2) Birefringence measurements under the above conditions.
(3) Stress measurements under the above conditions.
(4) Rate of crystallization studies under the above conditions.
(5) Microscopic observations of morphology changes occurring under the above conditions.
(6) Photographic light scattering observations of these morphological changes.
(7) Observations of mechanical and optical properties of films produced by crystallizing under the above conditions.

These studies are being made on films which are crosslinked with radiation of different doses, at different temperatures and at different elongations.

Contractor:	Materials Research Corporation, Orangeburg, New York
Contract Number:	AT(30-1)-2980
Present Contract Term:	April 1, 1963 through March 31, 1964
Cost to AEC:	$42,000
Contract Title:	SINGLE CRYSTAL PREPARATION BY FLOATING-ZONE ELECTRON BEAM MELTING
Investigators:	Gerald Abowitz

Scope of Work:

Single crystals of high purity iron 0.090 ins. in diameter and up to 3 ins. in length can now be grown by the strain anneal technique.

The primary goals of the present program is to further improve the quality of the single crystals already being produced, and to extend the present technique to the growth of both larger single crystals and crystals in sheet form. In addition, further purification of the starting material will be attempted. The methods which will be investigated are electrolytic migration and ultra high vacuum annealing.

The second and final phase of the proposal is restricted to an investigation of the structural perfection of the grown crystals. Methods by which the substructures will be investigated are etch-pits, dislocation decoration, diffractometer studies of the peak broadening and double crystal diffractometry.

Contractor: Mellon Institute, Pittsburgh, Pennsylvania

Contract Number: AT(30-1)-2684

Present Contract Term: November 1, 1962 through October 31, 1963

Cost to AEC: $126,732

Contract Title: ALLOYS OF THE NOBLE METALS

Investigators: T. B. Massalski

Scope of Work:

This project is concerned with experimental research in the general field related to the phase stability, electronic structure and physical properties of alloys based on the noble metals. The following aspects are under study at present:

(1) X-Ray investigations of accurate lattice spacings and of stacking faults - Accurate lattice spacings are being measured systematically within the phase fields of several close-packed hexagonal intermediate phases. The current research involves measurement at room temperature in the binary systems Cu-Zn, Ag-Cd, Ag-Zn, Au-Zn, and Cu-Ga and ternary systems Au-Cu-Ge and Au-Cu-In. In addition changes of lattice spacings with temperature are being studied in the system Cu-Ge. In both cases the principal aim has been the study of the relationship between the lattice spacings and the electronic structure.

Stacking fault probability measurements, following deformation by filing, are being carried out in the binary systems Ag-Cd, Au-Cu, Cu-Ag, and Ag-Au.

(2) Phase transformations - Metallographic, dilatometric and X-ray methods are being used to study the progress and the crystallographic features of transformations which occur upon quenching in the system Cu-Ga. The 'massive' type of transformation is being studied in particular detail by means of hot-stage microscopy.

(3) Electronic specific heat - At present no satisfactory theory is available for the changes with composition of the electronic specific heat in alloy systems. The scope of this program is to obtain systematic data for several alloy systems based on the noble metals and to relate the data to the density of states at the Fermi level. The current investigation covers alloys in the Cu-Zn system.

(4) Deformation characteristics of intermediate phases - The temperature dependence of the critical resolved shear stress and other deformation parameters are being studied in single cyrstals of close-packed hexagonal alloys in the Cu-Ge system which possess the ideal axial ratio. These studies are related to the measurements of lattice spacing changes with temperature in the same system.

Recent Publications:

H. W. King, and T. B. Massalski, "Lattice Spacings Relationships and the Electronic Structure of H.C.P. Phases Based on Silver," Phil. Mag., 6, (1961) p. 669.

T. B. Massalski and H. W. King, "Alloy Phases of the Noble Metals," Prog. in Materials Sci., 10, (1961) p. 1-78.

H. W. King and L. F. Vassamillet, "Precision Lattice Parameter Determination by Double-Scanning Diffractometry," Applications of X-Ray Analysis, Plenum Press, 1961.

G. F. Bolling, T. B. Massalski, and C. J. McHargue, "An X-Ray Study of Deformation Stacking Faults at Low Temperatures in Lead, Some Lead Alloys, and Aluminum," Phil. Mag., 6, (1961) p. 491.

L. F. Vassamillet, "Stacking Fault Probability of Noble Metal-Zinc Alloys," J. Appl. Phys., 32, (1961) pp. 778-782.

H. W. King and T. B. Massalski, "Structural Transformations in Ag-50 at .% Zn Alloy," Trans. A.I.M.E., accepted for publication.

T. B. Massalski and J. Kittl, "Discussion on the Eutectoid and Massive Transformations - Symposium on the Decomposition of Austenite, Interscience Publications, New York, To be published.

H. W. King and S. G. Glover, "The Influence of Alloying Elements on the First Stage of Tempering in High-Carbon Steels," J. Iron Steel Inst., 196, (1960) pp. 281-288.

J. E. Kittl and T. B. Massalski, "The Use of CuK Radiation for Detection of Order in Cu-Zn and Cu-Ga Alloys," J. Appl. Phys., Accepted for publication.

T. B. Massalski, "Meteorites and Cosmology in the Light of Recent Research, Revista Miniera, Geologia y Mineralogia, Buenos Aires, 25, (1961) p. 56.

T. B. Massalski, "Some Metallurgical Aspects in the Study of Meteorites," Arizona Meteorite Symposium, J. Wiley and Sons, Accepted for publication.

Contractor:	Michigan College of Mining and Technology Houghton, Michigan
Contract Number:	AT(11-1)-916
Present Contract Term:	June 15, 1962 through June 14, 1963
Cost to AEC:	$26,248
Contract Title:	STRUCTURE AND PROPERTIES OF SOLID SOLUTIONS
Investigators:	A. A. Hendrickson

Scope of Work:

The main objective of this research is to determine the cause or causes of strengthening in solid solutions. The experimental work includes the measurement of (1) The effect of growth procedure on yield strength, (2) the yield strength as a function of strain rate and temperature, and (3) yield point phenomena from strain aging. The solid solutions under investigation include face centered cubic solid solutions based on silver and substitutional solid solutions of body centered cubic refractory metals. The mechanical testing is done on single crystals in tension with the test temperatures varying between 4.2° and 500°K; the strain rate range is from 10^{-5} to 10^{-3} per second. The experimental results are utilized to evaluate current theories of solid solution strengthening.

Recent Publications:

G. E. Tardiff and A. A. Hendrickson, "Yield Points in Ag Base Zn Solid Solutions" Accepted by Acta Met.

A. A. Hendrickson, "Solute Segregations to Stacking Faults" Accepted by Acta Met.

Contractor: Michigan State University, East Lansing, Michigan

Contract Number: AT(11-1)-400

Present Contract Term: May 1, 1962 through April 30, 1963

Cost to AEC: $10,050

Contract Title: THERMAL PROPERTIES OF SEPARATED METALLIC ISOTOPES

Investigators: D. J. Montgomery

Scope of Work:

As part of a program utilizing isotopic mass as a probe for the solid state, we have determined the temperature dependence of the relative electrical resistance of specimens of "isotopic alloys" made up of varying proportions of lithium-6 and lithium-7. To test the predictions based on these results, the absolute resistivity of these alloys is to be measured at room temperature.

Recent Publications:

D. J. Montgomery, E. H. Wintermute, and A. E. Smith, "Static Electrification of Filaments: Effect of Filament Diameter," Textile Research Jnl. 31, (1961) p. 25.

R. H. Misho and D. J. Montgomery, "Effect of Temperature on Infrared Absorption of Solid LiH and LiD," Bulletin of the Am. Phys. Soc. 6, (1961) p. 284.

D. J. Montgomery, "Bulk Properties of Stable Isotopes as a Probe for Liquid-State and Solid-State Investigations," Progress in Nuclear Energy, Series 5, Vol. 3, Metallurgy and Fuels, pp. 486-476. Pergamon Press, 1961.

R. H. Misho and D. J. Montgomery, "Effect of Isotopic Composition on Infrared Absorption Spectra of Lithium Hydride and Lithium Fluoride," Bulletin of the Am. Phy. Soc. 6, (1961) p. 450.

Contractor:	Michigan State University, East Lansing, Michigan
Contract Number:	AT(11-1)-1042
Present Contract Term:	June 1, 1962 through May 31, 1963
Cost to AEC:	$31,290
Contract Title:	GROWTH AND PROPERTIES OF METAL AND COMPOUND SINGLE CRYSTALS
Investigators:	Chuan T. Wei

Scope of Work:

The formation of imperfections, especially dislocations, during the growth of metal and compound crystals is being investigated, particularly with reference to the role of mechanical and thermal stresses. Attention is given to the development of techniques and equipment for the growth of crystals such that mechanical and thermal stresses are minimized. The effect of stresses during crystal growth is being evaluated with zinc and lithium fluoride, using x-ray and etch pit techniques to evaluate the dislocation content and arrangement in crystals grown with a minimum of thermal and mechanical stress.

The mechanism of dislocation generation during the development of deformation bands in zinc will be studied by using x-ray techniques to observe the movement and arrangement of dislocations before and after stressing the most perfect crystals which can be prepared.

Crystals may be subjected to tests to determine the existence of any unusual mechanical or physical properties, and to elucidate the role of dislocations in determining properties.

Contractor: Michigan State University, East Lansing, Michigan

Contract Number: AT(11-1)-1247

Present Contract Term: February 1, 1963 through January 31, 1964

Cost to AEC: $16,076

Contract Title: STUDIES OF CONDUCTIVITY OF THIN METALLIC WIRES

Investigators: F. J. Blatt

Scope of Work:

Measurements of the resistivity of thin wires (diameter < mfp) at low temperatures have shown that not only the residual but also the temperature dependent resistivity increases with decreasing wire diameter. An explanation for these observations was provided by Blatt and Satz who showed that the additional size-and-temperature dependent resistivity is the result of diffuse surface scattering of electrons which are brought to the surface by small angle electron-phonon scattering. The theoretical expression contains only one parameter, the ratio of Normal-to-Umklapp electron-phonon scattering in the bulk metal. The present research program calls for the measurement of resistivity in the normal state of thin wires of lead, tin, indium and possibly other metals between $1.2^{\circ}K$ and $4.2^{\circ}K$. We anticipate the observation of a size-and-temperature dependent resistivity which should allow us to estimate the relative importance of Normal and Umklapp scattering. These estimates will be compared to others based on thermoelectric data where available. We also plan to measure the magnetoresistance of our thin wire specimen to fields of 20 kgauss since qualitative arguments suggest that the magnetoresistance coefficient should also be a function of wire size. Finally, we intend to develop a computer program for calculating normal and Umklapp scattering contributions to the ideal resistivity for metals with known, nonspherical Fermi surfaces so that we may make a meaningful comparison of experimental results and theory.

Contractor:	Michigan, University of, Ann Arbor, Michigan
Contract Number:	AT(11-1)-543
Present Contract Term:	June 1, 1962 through May 31, 1963
Cost to AEC:	$33,900
Contract Title:	INVESTIGATION OF THERMODYNAMIC ACTIVITIES AND SOLUBILITY RELATIONSHIPS IN BISMUTH SYSTEMS
Investigators:	Richard E. Balzhiser

Scope of Work:

The purpose of the study is to:

1. Investigate optical absorption techniques for pressure determination in metallic vapors and to use these to determine thermodynamic properties.

2. Investigate interactions in liquid metallic systems using solubilities and dissociations of compounds such as uranium carbide in the metallic systems as the experimental technique.

Optical absorption work has been done on pure bismuth, U-Bi, and Bi_2Te_3. The free energy of formation of uranium carbide at 800°C has been calculated from measured dissociation of the carbide in bismuth.

Work on interaction of uranium with other solutes in bismuth has been continued. A study of the interaction of lead in aluminum has been started.

Contractor:	Michigan, University of, Ann Arbor, Michigan
Contract Number:	AT(11-1)-771
Present Contract Term:	May 1, 1962 through April 30, 1963
Cost to AEC:	$25,000
Contract Title:	TRANSPORT PROPERTIES OF LIQUID METALS
Investigators:	Edward E. Hucke

Scope of Work:

This project is concerned with measuring the electric mobility of solute atoms in liquid metals. Accurate measurements of mobility are being made in the system Bi-Sn as a function of temperature and composition. Attempts are being made to correlate the mobility measurements with thermodynamic properties. Diffusion potential measurements are being attempted for use with the mobility data to verify the Onsager reciprocity relations.

Contractor: Michigan, University of, Ann Arbor, Michigan

Contract Number: AT(11-1)-979

Present Contract Term: March 1, 1962 through February 28, 1963

Cost to AEC: $32,350

Contract Title: THE THERMODYNAMIC PROPERTIES OF LIQUID METALLIC SOLUTIONS

Investigators: Robert D. Pehlke

Scope of Work:

The purpose of this research project is to extend the experimentally determined data on binary and ternary liquid metallic solutions, and to utilize them in determining the applicability of current theory in predicting the thermodynamic properties of liquid metallic solutions.

The work undertaken during the coming year will consist of:

1. Extend measurements by high temperature galvanic cells on zinc with third elements in liquid tin, measure the interaction between zinc and tin in liquid lead, and between copper and zinc in liquid bismuth.

2. Extend the measurements by high temperature galvanic cell on the uranium activity of liquid bismuth to the effect of third element addition and to the uranium activity in dilute solution in other solvent metals.

3. Complete the study of the interaction between hydrogen and dissolved solutes in liquid cobalt and extend these measurements to liquid nickel as a solvent metal.

4. Complete the study of the interaction between nitrogen and dissolved solutes in liquid cobalt.

5. Examine possible theoretical models for correlating interaction parameters in liquid metallic solutions.

Recent Publications:

R. D. Pehlke, "Interaction Parameters in Dilute Molten Alloys," Acta Met. (1962).

Contractor: Michigan, University of, Ann Arbor, Michigan

Contract Number: AT(11-1)-1086

Present Contract Term: October 1, 1962 through September 30, 1963

Cost to AEC: $12,134

Contract Title: THE OXIDATION OF THIN SINGLE CRYSTALS OF NICKEL

Investigators: L. O. Brockway

Scope of Work:

Previous work in this laboratory has shown that thin (700 Å) films of copper and nickel prepared by condensation onto heated sodium chloride surfaces can be treated to produce widely varying densities of stacking faults and dislocations. Films annealed in hydrogen at 600°C while still mounted on the sodium chloride show many stacking faults with an average width of about 2.0×10^{-4} cm; films annealed only after removal from the sodium chloride show no stacking faults but many dislocations amounting to about 10^9 per square centimeter. The variations in the annealing technique afford some control of the type and density of imperfections. A further control of dislocations is afforded by the introduction into the metal film of traces of impurity atoms.

The present work deals mainly with the preparation of copper films doped with small amounts of tellurium and annealed variously to produce different densities of stacking faults and dislocations. In the subsequent oxidation the oxide nucleation sites, and the size and epitaxial arrangement of the oxide particles are observed by electron microscopy and diffraction.

Contractor: Western Reserve University, Cleveland, Ohio

Contract Number: AT(11-1)-1108

Present Contract Term: November 15, 1962 through November 14, 1963

Cost to AEC: $31,000

Contract Title: ELECTRONIC SPECIFIC HEAT OF ALLOYS

Investigators: Ben A. Green, Jr.

Scope of Work:

The purpose of this work is to measure the specific heat of dilute silver-based solid solutions in the liquid helium range of temperatures. The electronic contribution may be separated from the lattice contribution to the specific heat allowing one to determine (1) the density of electron states at the Fermi level of the alloy and (2) the Debye temperature of the lattice.

A calorimeter is used which incorporates the following features:

(1) The sample is mounted ridgidly by means of nylon screws. This introduces an appreciable, but constant, heat leak into the sample. Specific heats are then determined dynamically.

(2) A mechanical heat switch of simple construction replaces the usual helium exchange gas.

(3) The germanium resistance thermometer is permanently mounted in the calorimeter and need not be heated or handled when changing samples.

In the dynamic method of measuring specific heats, the heat input is caused to vary as a square wave whose mean height determines the average temperature at which the measurement will be made. The temperature varies as a triangular wave whose slope divided into the amplitude of the input heat wave yields the heat capacity.

The results on densities of states will be compared to Rowland's recent measurements based on the Knight shift.

Contractor: Western Reserve University, Cleveland, Ohio

Contract Number: AT(11-1)-1146

Present Contract Term: March 1, 1963 through February 29, 1964

Cost to AEC: $42,000

Contract Title: RECOIL-FREE SCATTERING OF GAMMA RAYS

Investigators: John K. Major

Scope of Work:

The recoil-free scattering of gamma rays from solids and liquids will be studied as a function of temperature, by using the Mössbauer effect as an energy analyzer. Phase transitions between the solid and liquid states will be studied, and the relative amounts of recoil-free scattering fromlinear and cross-linked polymers will be measured. From determinations of the Debye-Waller factor, an effective Debye temperature will be deduced as a function of the scatterer temperature, yielding information on the phonon excitation spectrum not otherwise readily available. Information on the self-diffusion coefficient will be obtained from determinations of the line width of the recoil-free scattering. The importance of local order and, in particular, molecular, molecular linkage in making recoil-free scattering possible will be explored in these experiments. In addition, recoil-free resonant absorption and scattering in Tm^{169} will be studied.

Contractor: Western Reserve University, Cleveland, Ohio

Contract Number: AT(11-1)-1297

Present Contract Term: June 15, 1963 through June 14, 1964

Cost to AEC: $40,000

Contract Title: POSITRON ANNIHILATION IN LIQUIDS AND SOLIDS

Investigators: John D. McGervey

Scope of Work:

This is a new contract in which four problems involving positron annihilation in condensed systems are being attacked:

1) It has been found that solute atoms in aqueous solutions shorten the mean lifetimes of the positrons injected into these solutions. The mechanism by which this occurs is still uncertain but DeBendetti and McGervey have suggested that this effect arises from capture of the electron from positronium, leaving a free position which has a much shorter life than positronium. Further study of this phenomenon is being made with the objective of elucidating the mechanism of positronium destruction.

2) It has recently been observed that the application of an electric field lessens the fraction of positrons involved in positronium in solids, but does not affect the lifetime of positronium. This is the opposite effect of an electric field on positronium "atoms" in gases and the reason for the effect in solids is not yet apparent. Further study of this along with parallel studies of the effect of an electric field on the life of free positrons is being conducted.

3) Recent advances in the precision of mean life measurements have made it possible to measure mean lives of positrons in metals by direct measurement of the logarithmic slope of the decay curves. This is important because data in the literature show wide disagreement. Lifetimes in a large group of metals are being determined by measuring the slopes of the decay curves, and cases in which a long lived component is present are being sought.

4) The angular correlation of the gamma ray photons emitted from annihilation events can be used to determine the momentum distribution of the electrons taking part in these events. It is hoped that further development of this technique and the use of single crystal samples will make it possible for the data to be applied to the mapping of Fermi surfaces. This sort of work is continuing.

Contractor: Westinghouse Electric Corporation, Pittsburgh, Pennsylvania

Contract Number:

Present Contract Term:

Cost to AEC: $39,977

Contract Title: REACTIONS OF HYDROGEN WITH ALLOYS OF ZIRCONIUM

Investigators: Earl A. Gulbransen

Scope of Work:

The influence of alloying on the absorption of hydrogen into zirconium is being studied. One purpose of this investigation is to learn more about a periodicity of hydrogen uptake with alloying species which has been observed by U.K.A.E.A. scientists. The present investigators postulate that the phenomenon has its origin in the properties of the intermetallic compounds present in the zirconium alloys studied because of the very low solubility of the solute elements in question in alpha zirconium.

The eutectoid and the first intermetallic compound composition will be studied in binary alloys of Zr with V, Cr, Fe, Co, Ni, Cu and Mo.

Contractor: Wisconsin, University of, Madison, Wisconsin

Contract Number: AT(11-1)-987

Present Contract Term: February 1, 1963 through January 31, 1964

Cost to AEC: $21,880

Contract Title: DEFECT PHASES IN ALLOYS

Investigators: Richard A. Dodd

Scope of Work:

The supposed existence of defect structures, containing high concentrations of vacant lattice sites, in primary solid solutions is being investigated by examination of possible discrepancies between actual and theoretical densities. Such defect structures have been reported in Al(Zn), Al(Mg), Au(Ni), Ag(Zn), and Sn(In). It has already been shown that the first three of these phases do not in fact contain high concentrations of vacancies, and that solidification microporosity caused the reporting of erroneous results.

The probable existence of defect structures in the 21/13 electron compounds, gamma Ni-Zn and gamma Au-Zn, is also being examined by the method of density discrepancies. These alloys are being prepared by vapor diffusion of zinc into γ (Ni-Zn) and γ(Au-Zn) alloys which solidify at fixed temperatures. This method obviates all errors due to solidification microporosity, and will enable the defect concentrations to be precisely evaluated.

Subsequently, the effect on diffusion rates and mechanical properties of vacancies due to Brillouin zone effects will be investigated. This work will involve γ(Au-Zn) and γ(Ni-Zn) following the measurements of vacancy concentrations in these alloys. Although the effect of non-equilibrium vacancy concentrations (due to plastic deformation, irradiation, or quenching) on diffusion, strength, plastic deformation, etc., has been studied repeatedly, the effect of vacancies on zone effects has received little or no attention.

Contractor: Yale University, New Haven, Connecticut

Contract Number: AT(30-1)-2560

Present Contract Term: April 1, 1963 through March 31, 1964

Cost to AEC: $19,488

Contract Title: X-RAY STUDY OF THE STRUCTURE OF LIQUID METALS AND ALLOYS

Investigators: C. N. J. Wagner

Scope of Work:

A theta-theta diffractometer (fixed horizontal sample, x-ray tube and detector both movable with same angular speed towards or away from each other) is being used to study the liquid alloys of Hg-Tl, dilute mercury alloys with Pb, Sn, Bi, In, Zn, and Cd, and Ag-Sn. Recent advances in the x-ray theory of binary liquids make it possible to study systems with elements of largely different scattering factors. It is planned to investigate Au-Sn, Pb-Sn, and In-Sn, after completion of the work on the mercury alloys and Sn-Ag.

Contractor: Yale University, New Haven, Connecticut

Contract Number: AT(30-1)-2723

Present Contract Term: January 1, 1963 through December 31, 1963

Cost to AEC: $18,394

Contract Title: THE STRUCTURE AND ASSOCIATED PROPERTIES OF IONIC SOLID SOLUTIONS

Investigators: W. D. Robertson

Scope of Work:

The objective of the present program of research is threefold:

First, a study of the physical and chemical factors that determine the range of solid solubility. Experimentally, the solubility limit in sodium chloride of the chlorides of the elements from groups I and II of the periodic table is being determined, as a function of temperature and composition. An essentially automatic differential thermal analysis technique is being used as a primary source of information, together with high temperature x-ray diffraction and high temperature microscopy.

Second, an investigation of the mechanism and kinetics of precipitation from ionic solutions will be made, using the information obtained from the solubility studies and with special emphasis on the role played by crystal defects. A hot stage microscope, capable of temperatures up to 1000°C and suitable for both transmitted and reflected polarized light is being assembled for this work.

Third, an investigation of defect concentrations in ionic solid solutions, as measured by the difference between macroscopic and x-ray densities is being made in the system $LiF-MgF_2$ for which the phase diagram has recently been redetermined.

Contractor: Yale University, New Haven, Connecticut

Contract Number:

Present Contract Term: June 1, 1963 through May 31, 1964

Cost to AEC: $124,200

Contract Title: THE STUDY OF IDEAL MAGNETIC CRYSTALS

Investigators: Werner P. Wolf

Scope of Work:

This is a new program concerned with investigation of magnetic materials, chosen to be as ideal and simple as possible, in order that their properties may be understood in detail. The principal results to be expected from this investigation are a greater understanding of the physical processes governing the properties of magnetic materials, and the discovery of new types of magnetic materials. In outline, the program will be concerned with the following subjects.

1) Preparation of Materials

   a) Preparation of known compounds by standard techniques. (e.g. $Dy_3Al_5O_{12}$ and other Ga and Al garnets)
   b) Search for new materials
   c) Growth of single crystals of interesting materials.

2) Study of Interactions and Magnetic Phase Transitions at Low Temperatures

   a) Precision low field susceptibility measurements.
   b) Magnetization measurements in larger fields.
   c) Thermal measurements.
   d) Irreversible and time dependent effects.

3) Experiments and Temperatures below $0.3^{\circ}K$

   a) Techniques of magnetic cryogenics.
   b) Study of magnetic ordering at very low temperatures.

4) Electron Spin Resonance

   a) Resonance of magnetically isolated ions.
   b) Resonance of pairs of ions.
   c) Ferromagnetic and antiferromagnetic resonance.

Contractor: Tennessee, University of, Knoxville, Tennessee

Contract Number: AT(40-1)-1068

Present Contract Term: September 1, 1962 through August 31, 1963

Cost to AEC: $8,964

Contract Title: APPLICATION OF ADIABATIC CALORIMETRY TO METAL SYSTEMS

Investigators: E. E. Stansbury

Scope of Work:

The broad scope of this research is the application of dynamic adiabatic calorimetry to the measurement of specific heats and related thermal effects of metal systems in the temperature range extending from room temperature to 1000°C. With the present calorimeter specific heats can be measured with a reproducibility of about ±0.5 per cent up to 700°C.

The current emphasis has been on determination of the specific heat behavior of binary solid solutions for various histories (e.g., quenching effects, neutron irradiation). A study of the effect of heating rate and neutron irradiation on the specific heat of an aluminum- and a gallium-copper solid solution has been completed. An anomalous behavior is observed which is associated with short-range disordering. A study of the effect of quenching from high temperatures for these two alloys is about complete; the results indicate that the behavior is strongly influenced by the presence of quenched-in vacancies.

A detailed study of the specific heat of a titanium-hydrogen alloy near the eutectoid composition has been undertaken and the major portion is complete. Correlation of this information with other experimental approaches should clarify the equilibrium situation and also kinetic effects observed in this system.

Further investigations of the specific heat behavior of binary copper-base solid solutions is being undertaken, including alloys containing silicon, germanium, manganese, and arsenic. Also preliminary results have been obtained on binary nickel-base solid solutions containing molybdenum and chromium, both of which also show anomalies similar to that of the copper-base alloys.

Contractor: Toledo, University of, Toledo, Ohio

Contract Number: AT(11-1)-1000

Present Contract Term: February 1, 1963 through January 31, 1964

Cost to AEC: $12,343

Contract Title: OXIDATION OF ZIRCONIUM-NIOBIUM ALLOYS IN THE TEMPERATURE RANGE 300-500°C

Investigators: Otto Zmeskal

Scope of Work:

The purpose of this project is to investigate the mechanism of the oxidation of zirconium-niobium alloys in the low temperature range.

An investigation will be made into the effect of total pressure on the oxidation process. Regular, smooth oxidation curves at low temperatures have been obtained by others only under conditions of low total pressure. The results of the present investigation show great irregularity at 400°C, a phenomenon displayed in many repeat runs, and have convinced us that this is a matter worth investigating.

The metallographic examinations will be continued and elaborated upon to follow the visual sturctural changes during the oxidation process. The change in character of the interface from a straight one to a very irregular one is an interesting phenomenon. Surface studies will throw light on the cracking that develops in the film.

Study will also be made of the development of thin oxide films on Zr and Zr-Nb alloys at low temperatures (i.e. 500°C or lower) by means of an electron microscope. It is hoped that the results from the electron micrographic examination of the films will contriuute to the explanation of the irregular behavior at low temperatures.

Contractor: Tufts University, Medford, Massachusetts

Contract Number: AT(30-1)-2968

Present Contract Term: May 1, 1963 through April 30, 1964

Cost to AEC: $11,500

Contract Title: THOMAS-FERMI MODEL FOR GRAPHITE

Investigators: George Handler

Scope of Work:

Since a vastly improved basis set for generalized Thomas-Fermi theory has been found as a result of the first year's work, it is planned to exploit this result in the following ways:

1) in a diatomic molecular problem, H_2^+

2) in a self-consistent field calculation for larger atoms.

The improved TF theory shows every promise of being equivalent to a second-order treatment, without the attendant complications.

In addition, we plan to investigate the effect of symmetrization on the approximate first order density matrix of Thomas-Fermi theory.

Contractor:	Union Carbide Corporation, Cleveland, Ohio
Contract Number:	AT(30-1)-2051
Present Contract Term:	April 1, 1962 through March 31, 1963
Cost to AEC:	$33,284
Contract Title:	PREPARATION OF SEMICONDUCTING MATERIALS
Investigators:	R. D. Westbrook

Scope of Work:

The objective of this work is to provide USAEC contractors with carefully characterized high quality semiconductor crystals prepared to precise specifications. Single crystals of silicon, germanium, and indium antimonide are grown especially to meet unusual requirements as to purity, nature and degree of doping, dislocation density, etc., as requested by USAEC contractors. The crystals so produced are carefully studied both by physical and chemical methods to insure that the specifications have been met. This crystal growing service can be extended to include other semiconducting materials.

Contractor: Utah, University of, Salt Lake City, Utah

Contract Number: AT(11-1)-1122

Present Contract Term: December 1, 1962 through November 30, 1963

Cost to AEC: $12,500

Contract Title: RECRYSTALLIZATION AND SINTERING OF OXIDES

Investigators: Ivan B. Cutler

Scope of Work:

Work is being done in the four areas of (1) the rate of shrinkage of powder compacts, (2) the electrical conductivity of oxide systems, (3) the kinetics of impurity diffusion, and (4) normal grain growth of polycrystalline oxides. Research to be done in each of these four areas is described briefly as follows:

(1) The effect of several impurities on the shrinkage rate of alumina will be determined. Impurities selected will be those known from experience to have an effect on the initial stages of sintering. It is expected that from the consideration of the valence of the impurity added, some inference will be made concerning the mechanism of grain boundary on bulk diffusion, as the case may be found during analysis of the shrinkage isotherm.

(2) It has already been found in the phase of the work just concluded that electrical conductivity of magnesia doped with iron oxide may be correlated on the basis of the Heikes hopping mechanism. The resistance was found to be a function of the hopping distance as well as the number of carriers available to hop. It is proposed that this phenomenon be studied further, at even more dilute concentrations of impurities and with alumina as well as magnesia. It will be possible by going from high impurity concentrations to dilute impurity concentrations to see how far the hopping mechanism may be applied to the electrical conductivity of oxide materials.

(3) Analysis of data obtained on the phase of the project just concluded shows that the entropy of activation is markedly influenced by the concentration of the vacancies introduced by the impurity on the impurity diffusion. These studies will be extended to other systems to discover the cause for the unusual effect of vacancy concentration of the activation entropy. Systems to be studied are cobalt oxide and nickel oxide diffusing into magnesia, and FeO and Fe_2O_3 into single crystals of alumina.

(4) Bagley has established that sodium oxide impurity brings about exaggerated grain growth in alumina. MgO is added by some investigators to inhibit grain growth so that fine-grained alumina can be produced. Apparently magnesia acts to form spinel as a second phase. This is believed to retard the growth of the grain boundaries. Further, grain growth theory predicts a square root of time dependence. This holds in magnesia and calcia. In alumina, a cube root of time dependence is apparently obtained. This is not well understood. This may be a function of impurity content. These phenomena are being studied further experimentally.

Recent Publications:

A. U. Daniels, Jr, R. C. Lowrie, Jr., R. I. Gibby, and I B. Cutler, "Observation on Normal Grain Growth of Magnesia and Calcia" J. of The American Ceramic Society, Vol. 45, #6, (1962).

R. Shelley, E. B. Gibby and I.B. Cutler, "Note on Diffusion of Cobalt Oxide and Ferrous Oxide in Polycrystalline," J. of American Ceramic Society, Vol 45, #6. (1962)

Contractor: Utah, University of, Salt Lake City 12, Utah

Contract Number: AT(11-1)-1284

Present Contract Term: April 15, 1963 through August 14, 1964

Cost to AEC: $21,917

Contract Title: A MAGNETIC RESONANCE STUDY OF DEFECTS IN SOLIDS

Investigators: William D. Ohlsen

Scope of Work:

The role of the hyperfine interaction in low-temperature spin-lattice relaxation will be experimentally studied by observing the effects of carbon isotopic substitution on the liquid-helium-temperature relaxation time of paramagnetic radiation-damage centers in Calcite. The effects sought will be a hyperfine lattice-coupling increase in the relaxation rate and, for high defect densities, a reduction due to hyperfine line broadening in the spin diffusion rate. The hyperfine interaction information will also be used to study the structures of the Calcite radiation damage centers. Electron irradiation will be used for defect production with the initial work involving room temperature irradiations and later work using low-temperature irradiations.

A study of second-order-quadrupole NMR-line shifts in mixed alkali-halide crystals will be continued. With KBr discrete Br lines quadrupole shifted by Na impurities have been seen and measured. The interpretation of these results is so far incomplete since the patterns obtained do not seem to agree with those which should result from simple Br sites such as (100) or (111) with respect to the Na. The amount of the rotation pattern which can be seen is limited by the width of the large central line resulting from unshifted Br. Attempts will be made to reduce the central-line width by annealing the samples. Similar experiments will also be run on NaBr doped with K.

Contractor: Vanderbilt University, Nashville, Tennessee

Contract Number: AT(40-1)-3091

Present Contract Term: March 1, 1963 through February 29, 1964

Cost to AEC: $17,000

Contract Title: DEFORMATION STUDIES OF SUPERLATTICE STRUCTURE

Investigators: J. J. Wert

Scope of Work:

It is known that the strength properties of a superlattice type alloy subjected to plastic deformation change at different rate than those associated with an initially disordered alloy. In general, it is believed that deformation will create new domain boundaries and destroy order through movement of dislocations on intersecting planes. Thus the effect of deformation is to decrease the domain size present in an alloy. Cohen and Bever of MIT have found that the Knoop hardness and yield strength of an initially order specimen increased more rapidly than that of initially disordered specimen as a function of plastic deformation. Presumably, the change in antiphase domain size due to plastic deformation enhances the materials resistance to plastic deformation. This investigation is designed to study the effects of deformation on Cu_3Pt in the ordered and disordered states in terms of the strain distribution in different crystallographic directions, the antiphase domain size and the particle size present as function of plastic deformation, and hence, the degree of order present. X-ray diffraction data will be analyzed via the method described by Averbach and Warren and will be correlated with mechanical properties wherever possible. It is anticipated that this investigation will yield fundamental knowledge concerning the deformation of superlattice structures.

Contractor: Vermont, University of, Burlington, Vermont

Contract Number: AT(30-1)-3000

Present Contract Term: June 1, 1962 through September 30, 1963

Cost to AEC: $23,153

Contract Title: ABSORPTION OF HYDROGEN AND DEUTERIUM BY PALLADIUM-RICH ALLOYS

Investigators: T. B. Flanagan

Scope of Work:

The absorption of hydrogen (and deuterium) by a series of palladium-rich alloys are being studied below 100°C. An electrochemical approach is employed since it is difficult to obtain equilibrium absorption data below 100° using conventional gas phase techniques.

Theremodynamic parameters of absorption are being determined for each series of alloys and these parameters related to the percentage of added metal Isobars are being determined for both hydrogen and deuterium, i.e., the equilibrium concentration of absorbed hydrogen and deuterium at one atmosphere pressure as a function of temperature.

An investigation of the absorption of deuterium by a series of plantinum/palladium alloys is being completed. The heats, free energies and isotherms of absorption have been determined. Changes of electrical resistance with deuterium content have been determined for the series of platinum/palladium alloys. Results are compared with previous studies of hydrogen absorption by these alloys.

An isotopic selectivity in the absorption of hydrogen isotopes has been observed in certain platinum/palladium alloys, e.g., 8.80 and 12.00 per cent platinum (atomic per cent). This difference in isotopic solubilities has been utilized to remove preferentially hydrogen from heavy water-light water mixtures.

Research on the absorption of hydrogen by palladium-rich alloys is of interest in order to correlate the absorption properties with the nature of the added metal; these results may be a valuable aid in elucidation of the nature of the forces binding the hydrogen to the metal lattice.

Contractor:	Virginia Institute for Scientific Research Richmond, Virginia
Contract Number:	AT(40-1)-2860
Present Contract Term:	March 1, 1963 through February 29, 1964
Cost to AEC:	$12,435
Contract Title:	GROWTH OF SINGLE CRYSTALS OF BERYLLIUM FOR NEUTRON SPECTROMETERS
Investigators:	James F. Kirn

Scope of Work:

The objective of this contract is to develop a method for the growth of single crystals of beryllium of sufficient size, orientation and perfection to give satisfactory energy distribution for neutron monochronometers.

Small single crystals of beryllium have been grown previously. It is suggested that large, high purity crystals of 2.5" x4 and having a specific orientation will be needed for neutron spectroscopy. These assumptions will be examined by experiment. A technique will be developed for growing large single crystals and for seeding such crystals to the desired orientation.

Bridgman and Czochralski techniques of crystal growth will be used. Special emphasis will be placed on the pull technique which offers a method by which the crystal is grown free from crucible wall effects.

Contractor: Virginia Polytechnic Institute, Blacksburg, Virginia

Contract Number: AT(40-1)-2564

Present Contract Term: May 1, 1963 through April 30, 1964

Cost to AEC: $17,845

Contract Title: GOVERNING FACTORS IN THE FORMATION OF THE Cr_3O-TYPE STRUCTURE

Investigators: J. F. Eckel

Scope of Work:

The investigation of the V-Rh-Si and the Nb-Rh-Si systems is being continued. Alloys in the V-Rh-Si system are selected to test the extent of ternary solid solubility extending away from the 75 atom percent vanadium line corresponding to (A, B) V_3. Eight alloys containing 72.5 to 77.5 atom percent vanadium will be used. In the Nb-Rh-Si system, six alloys containing 72.5 to 77.5 atom percent niobium and up to 2.5 percent silicon are being used to determine if partial solid solubility exists between silicon and Nb_3Rh.

To investigate further the evidence that there is only limited solubility of the Group IV B-elements for the Group VIII B-elements, two systems, Nb-Rh-Sn and Cr-Rh-Si are being studied. All binary systems in the above ternary alloys form the Cr_3O-type structure. This investigation may also help to answer two other questions. First, does the solubility depend on the type of A-atom used, because solubility has been found only in the vanadium containing alloys? Secondly, do Group IV elements substitute for Group VIII elements in most cases when the Cr_3O-type compound occurs in both binary systems?

Contractor: Virginia Polytechnic Institute, Blacksburg, Virginia

Contract Number: AT(40-1)-2689

Present Contract Term: March 1, 1963 through February 29, 1964

Cost to AEC: $42,985

Contract Title: TEMPERATURE AND CRYSTAL STRUCTURE DEPENDENCE OF SPECIFIC HEAT, RESISTIVITY, MAGNETIC SUSCEPTIBILITY AND HALL EFFECT IN METALLIC CERIUM

Investigators: T. E. Lienhardt

Scope of Work:

The physical properties of cerium metal are being investigated in order to correlate anomalies observed in the temperature dependence of certain of the electrical, magnetic and thermal properties of the material with changes in its crystal structure. The electrical resistance of the metal as determined by temperature, crystal structure, and heating or cooling rates is being studied. Measurements of the thermoelectric force of cerium are being made between $4^{\circ}K$ and $300^{\circ}K$. The effects of thermal cycling and different cooling or warming rates on the value of the thermo-electric force are being investigated. Optical reflectance measurements are being made in the visible and infrared regions. A theoretical study is in progress to determine whether or not there is a relationship between anti-ferromagnetism and superconductivity and to evaluate the possibility of cerium becoming a superconductor.

Contractor: Virginia, University of, Charlottesville, Virginia

Contract Number: AT(40-1)-2488

Present Contract Term: February 1, 1963 through January 31, 1964

Cost to AEC: $66,765

Contract Title: PHYSICAL STUDIES OF THE SURFACE STATE

Investigators: John W. Mitchell and Nicolas Cabrera

Scope of Work:

Methods for producing crystallographic surfaces of (111) orientation on mechanically and chemically finished single crystals of copper and copper alloys are being developed. The study of the equilibration of copper surfaces by heating them in a mixture of argon and carbon tetrafluoride is therefore being actively pursued. These surfaces are being used for studies on the generation of dislocations at the surfaces. Etching and electron microscope methods are used for this work. New electrolytic methods have been worked out for producing etch pits at the points of intersection of dislocations with the surface and these have now been applied successfully to single crystals of copper aluminum alloys with up to 6 atom % of aluminum.

Single crystal ribbons of cadmium of high chemical purity and physical perfection are being strained with a tensile device in the electron microscope. The strain is determined from measurements made on the electron diffraction pattern. Some crystals have sustained elastic strains of greater than 4 % before failing by fracture. Attempts are being made to produce thin ribbons of silver for experimental work with the electron microscope on the role of the surface in yield phenomena.

The epitaxial overgrowth of nickel bromide upon chromic bromide will also be studied by electron diffraction and electron microscopic methods.

Recent Publications:

J. T. Bartlett and J. W. Mitchell, "Interactions between Dislocations with Burgers Vectors at 120° in Crystals of Silver Bromide," Philosophical Magazine, 6, (1961) p. 271.

Contractor: Virginia, University of, Charlottesville, Virginia

Contract Number: AT(40-1)-3012

Present Contract Term: June 1, 1963 through May 31, 1964

Cost to AEC: $26,970

Contract Title: AN INVESTIGATION OF VACUUM-DEPOSITED SINGLE-CRYSTAL SEMICONDUCTOR FILMS

Investigators: Avery Catlin

Scope of Work:

The proposed investigation is a continuation of research already in progress on the epitaxial growth of semiconductor films by vacuum deposition.

Films of germanium and silicon will be grown epitaxially on germanium and silicon substrates, and also on other substrate crystals such as calcium fluoride. Variables in the process of deposition which affect the crystalline perfection of the overgrown film will be studied, and the relationship between film deposition rates and substrate temperatures will be carefully examined.

The epitaxial techniques will be extended to deposition of semiconductor films on deposition metallic films, and the electrical properties of the resulting multilayer devices will be examined. The electrical properties of the junction formed by a deposited semiconductor will also be examined, and correlated with the crystalline perfection of the film and with the deposition techniques.

Contractor:	Virginia, University of, Charlottesville, Virginia
Contract Number:	AT(40-1)-3108
Present Contract Term:	June 15, 1963 through September 14, 1964
Cost to AEC:	$64,139
Contract Title:	INVESTIGATIONS ON THE BEHAVIOR OF POINT DEFECTS AND DISLOCATIONS
Investigators:	Doris Kuhlmann-Wilsdorf

Scope of Work:

Four problems constitute the scope of work:

a) By means of a recently developed, high sensitive density measuring apparatus, the volume of relaxation of vacancies may be measured. The concentration of vacancies and interstitials, and of their various aggregates, introduced into crystals through straining and by irradiation treatments will be measured using this technique.

b) Electrolytically deposited metal foils will be grown and examined with the ultimate aim to understand and control the propagation of crystal defects from a substrate into a growing crystal.

c) Using a special furnace, crystals will be grown at temperatures close to their melting point. These crystals will be studied to test theories on the origin of dislocations through vacancy condensation.

d) Employing the techniques of electrolytic deposition (point b. above) in which thin, distinguishable layers are introduced into foil crystals, the crystals will be stretched and an attempt to use the layers to map slip bands in three dimensions will be made.

This program is essentially a continuation of research formerly carried out at the University of Pennsylvania.

Contractor: Virginia, University of, Charlottesville, Virginia

Contract Number: AT(40-1)-3105

Present Contract Term: May 15, 1963 through May 14, 1964

Cost to AEC: $38,500

Contract Title: ELECTRONIC PROPERTIES OF METALS AND ALLOYS

Investigators: Robert V. Coleman

Scope of Work:

Experimental studies of the electric-magnetic properties of metals and alloys are to be carried out under this proposal. In particular, magnetoresistance and Hall effect measurements started under ONR contract (4176) will be continued and expanded. New experiments on the galvanomagnetic properties of single crystal thin films will also be started. Specific studies to be undertaken are:

a) Magnetoresistance in crystals of zinc, cadmium, magnesium, and their dilute alloys.

b) Magnetoresistance in single crystals of copper and silver and their dilute alloys.

c) Magnetoresistance in single crystal iron whiskers.

d) Hall effect studies to be correlated with the above magnetoresistance measurements.

e) Resistance, magnetoresistance, and Hall effect measurements on expitaxially grown single crystal films of metals.

Contractor: Virginia, University of, Charlottesville, Virginia

Contract Number: AT(40-1)-3109

Present Contract Term: May 1, 1963 through April 30, 1964

Cost to AEC: $24,560

Contract Title: THE EARLY PHASES OF REACTIONS OF GASES ON METAL SURFACES

Investigators: Kenneth R. Lawless

Scope of Work:

This proposed research comprises a program for the development of a low-voltage electron diffraction apparatus applicable to the specific problems of surface chemistry and its employment for investigation of the detailed character and chemical properties of crystalline metal surfaces. Past researches have indicated the complexity of processes occurring at the surface, by which chemical reaction is initiated, and the probable importance of certain detailed surface structures to the mechanisms involved. However, the techniques available and utilized heretofore have not been adequate to provide necessary detail, and have seriously limited the scope of the information secured.

It is believed that the newer developments in low-voltage electron diffraction now offer promise for detailed exploration of this important field. Following design and construction of the necessary high vacuum, low-voltage electron diffraction equipment, studies will be made of metal crystal surfaces; their structure on a "near atomic" scale; the cleanliness (freedom from foreign atoms) obtainable under experimental conditions; the phenomena involved at the metal-gas interface prior to attainment of steady-state, or equilibrium, conditions; and then similar studies of the mechanisms involved in the early phases of chemical reaction. Rates of reaction, sticking coefficients, and the structures of reaction products will be determined for several different crystal faces. Both high-voltage electron diffraction and electron microscopy will provide supplemental data on the structures.

Contractor:	Wake Forest College, Winston-Salem, North Carolina
Contract Number:	AT(40-1)-2413
Present Contract Term:	June 15, 1963 through June 14, 1964
Cost to AEC:	$14,467
Contract Title:	A STUDY OF ATOMIC MOVEMENTS IN SOLIDS EMPLOYING ANELASTIC MEASUREMENTS
Investigators:	Thomas J. Turner and G. P. Williams, Jr.

Scope of Work:

The Zener relaxation phenomena in substitutional solid solutions is being studied. A study of the Zener relaxation in the Ag/Au system has essentially been completed.

Attention is now being directed to the Zener relaxation in the Ag/Cd system and the exploration of the source of secondary relaxation peaks in the Ag/Au system. Work is also continuing on the effects of crystal orientation on Zener relaxation with the hope of obtaining information on the mechanism involved in the atomic motions to which this relaxation is ascribed. Measurements on lithium fluoride will also be carried out to obtain information on the nature and forces coming into play in the motion of atoms and dislocations.

Contractor: Washington, University of, Seattle, Washington

Contract Number: AT(45-1)-1375

Present Contract Term: March 1, 1963 through February 29, 1964

Cost to AEC: $19,537

Contract Title: PHASE TRANSFORMATION IN A EUTECTOID BINARY ALLOY SYSTEM

Investigators: Douglas H. Polonis

Scope of Work:

Ti-Cu alloys are being employed to determine the effect of alloy composition and tempering temperature on the decomposition of the substitutional martensite alpha-prime phase produced by quenching the alloys from the high temperature beta field. The tempering kinetics and decomposition mechanisms are being studied by x-ray techniques, microscopy and continuously monitored resistometric measurements which are being made at the tempering temperature. In particular, the relatively rapid decomposition of the martensitic alpha prime at the former beta boundaries is being studied:

(a) To determine the effect of tempering temperatures in the range 350°C-550°C on the morphology of the reaction products.

(b) To resolve the relative roles of nucleation and growth at different tempering temperatures.

(c) To discover the underlying reasons for the composition sensitivity of the boundary network reaction.

(d) To separate the contribution of this boundary reaction in the overall kinetics of the tempering reaction.

The potential role of quenched in lattice vacancies in the nucleation of Ti_2Cu from the alpha prime phase is also being carefully examined.

Alloys containing 1.5 wt.% copper can be made to yield, by quenching, either equi-axed supersaturated alpha or alpha prime. A study has therefore been initiated to investigate the effects of the morphology of these phases on the precipitation of Ti_2Cu.

Initial studies of the direct decompostion of the high temperature phases in binary eutectoid systems are now in progress and will continue during the year. The work is centered around the mechanisms and kinetics of the omega phase formation in Zr binary alloys.

Contractor: Wayne State University, Detroit, Michigan

Contract Number: AT(11-1)-1054

Present Contract Term: June 15, 1962 through June 14, 1963

Cost to AEC: $25,484

Contract Title: ELECTRON PARAMAGNETIC RESONANCE STUDIES OF RADIATION EFFECTS IN SOLIDS AND CHEMICAL COMPOUNDS

Investigators: Yeong-Wook Kim

Scope of Work:

The purpose of the present work is to study the nature of radiation damage to several selected solids and chemical compounds.

The work on lithium fluoride and several other lithium compounds, diphenyl picryl hydrazine, and chromium sequi-oxide will be further developed. An investigation will be initiated concerning possible effects of oxygen on the formation of radiation defects in selected organic compounds.

The investigations of the nature of radiation damage to these samples will be conducted by using the techniques of electron paramagnetic resonance absorption at controlled temperatures between 1.5°K and 600°K. If feasible and advantageous, the methods of electron-nucleus double resonance absorption and optical absorption will be additionally employed.

Neutrons, gamma-rays, and X-rays will be employed for the irradiation treatments.

It is also planned to vary, as far as possible, the temperature of irradiation, the temperature of sample, the species of nuclear isotope, the oxygen pressure, and the type of solvent.

Recent Publications:

Y.W. Kim and P. W. France, "Paramagnetic Resonance in Neutron-Irradiated $DPPH_2$," Bull. Am. Phys. Soc. Ser. II 6, (1961) p. 445.

Y. W. Kim and T. Bredin, "Paramagnetic Resonance in Neutron-Irradiated LiF at Elevated Temperatures," Bull. Am. Phys. Soc. Ser. II 7, (1962) p. 51.

Y.W. Kim and D. D. Hearn, "Electron Paramagnetic Resonance Absorption of Thermally Annealed Cr_2O_3 Below Curie Temperature," Appl. Phys. Letters, Vol. 2, No. 2, (1963) pp. 36-37.

Contractor: West Virginia University, Morgantown, West Virginia

Contract Number: AT(40-1)-2839

Present Contract Term: September 1, 1962 through August 31, 1963

Cost to AEC: $15,164

Contract Title: VOLUME MAGNETOSTRICTION IN FERROMAGNETIC MATERIALS

Investigators: Arthur S. Pavlovic

Scope of Work:

The overall objectives of this project is the measurement of the magnetostriction of ferromagnetic materials over a wide range of temperature and magnetic field strength and to attempt to interpret these results in terms of existing theories of ferromagnetism.

Specifically, the longitudinal and transverse magnetostriction of gadolinium has been measured. It is found that the magnetostriction is large and positive. The major contribution being a volume effect since the longitudinal and transverse magnetostriction do not differ by much. The measurements shall be extended to single crystals of gadolinium. Similar studies are being performed on dysprosium and magnetocaloric data will be obtained for both these rare earths.

The magnetostriction of iron and cobalt is being determined up to temperatures as close to their curie temperatures as possible.

Recent Publications:

S. H. Liu, "Indirect Exchange Theory of Ferromagnetism in Metals," Bull. Am. Phys. Soc. Series II, 7, (1962) p. 295.

E. R. Callen, "Static Magnetoelastic Coupling in Cubic Crystals," Bull. Am. Phys. Soc. Series II, 7, (1962) p. 263.

A. S. Pavlovic, W. E. Golemann, "Magnetostriction of Gadolinium and Dysprosium," Bull. Am. Phys. Soc. Series II, 7, (1962) p. 264.

Contractor:	Rensselaer Polytechnic Institute, Troy, New York
Contract Number:	AT(30-1)-3176
Present Contract Term:	March 1, 1963 through February 29, 1964
Cost to AEC:	$25,000
Contract Title:	PRECIPITATION PHENOMENA IN CERAMICS: THE SYSTEM $BaTiO_3$-$CaTiO_3$
Investigators:	Robert C. DeVries and George S. Ansell

Scope of Work:

It is proposed in this investigation to study the structure-property relationships in the binary system $BaTiO_3$-$CaTiO_3$ with particular emphasis on the precipitate structure, kinetics of precipitation, and the effect of the precipate on the change of capacitance with time. The structure-property relationships are based on the assumptions that change of capacitance is due to domain movement and that domains may be pinned by structural features such as a precipitate.

This investigation will involve the following parts:

a. preparation of solid solutions in the system;

b. heat treatment to form the precipitate;

c. measurement of the kinetics of the precipitation reaction;

d. description and interpretation of the precipitate-host structure;

e. measurement of change of capacitance with time in samples with and without the precipitate structure.

f. interpretation of the microstructure-property relationships.

Contractor:	RIAS, Baltimore, Maryland
Contract Number:	AT(30-1)-2531
Present Contract Term:	August 1, 1962 through July 31, 1963
Cost to AEC:	$30,407
Contract Title:	ELECTRON MICROSCOPE INVESTIGATION OF ALLOTROPIC TRANSFORMATIONS IN METALS
Investigators:	Henry M. Otte

Scope of Work:

The low temperature transformation in stainless steels is being investigated using primarily electron transmission microscopy. In a composition range around 18% Cr, 8% Ni, two structures (a bcc and an hcp) form martensitically; in those cases where the transformation can be made to go virtually to completion, the end product is the bcc structure. The question therefore arises: is the hcp structure a "metastable" intermediate phase in the transformation fcc to bcc, or is it merely a reflection of a low stacking fault energy of the fcc austenite? The answer to this could provide important information on the nucleation and the mechanism of the transformation.

Several approaches to the study of allotropic transformations are planned using mainly the electron microscope: (1) Observation of the formation of bcc martensite and hcp epsilon on cooling in the electron microscope, (2) Determination of the Burgers vectors of dislocations in the martensite, (3) Determination of the Burgers vectors of dislocations in the austenite - martensite interface.

A persual in greater detail of certain theoretical aspects is also to be considered, in particular: (4) the general theory of the resolution of an arbitrary strain into any prescribed number of invariant plane strains; (5) Consideration of the implication of recent experimental results on the determination of the direction of the homogeneous strain.

Related to allotropic transformations in general, the following are viewed as being within the scope of the project: (6) Factors affecting the nucleation and transformation of crystal structures in general; (7) The effect of radiation damage on allotropic transformations; (8) Correlation between physical and mechanical effects of allotropic transformations and the structural features observable by electron microscopy.

Recent Publications:

H. M. Otte, "Determination of the Dilatation Parameters in Martensitic Transformations," Acta. Cryst., 16, (1963) p. 8.

M. P. Drazin and H. M. Otte, "The Systematic Determination of Crystallographic Orientations from Three Octahedral Traces on a Plane Surface," Physica status solidi, 3 (1963)

Contractor: Stanford University, Stanford, California

Contract Number: AT(04-3)-283

Present Contract Term: May 1, 1962 through July 31, 1963

Cost to AEC: $30,167

Contract Title: THERMODYNAMIC AND TRANSPORT PROPERTIES IN LIQUID METAL SOLUTIONS

Investigators: David A. Stevenson

Scope of Work:

Thermodynamic Studies - Thermodynamic studies are directed toward the experimental determination of excess partial molar enthalpy and entropy values in dilute binary liquid metal solutions. The experimental approach employed is the determination of the distribution between solid and liquid phases in systems where the solid phase is essentially a pure metallic element. This experimental information may then be treated by solution thermodynamics to give the excess quantities mentioned above. The systems aluminum-cadmium and aluminum-bismuth are currently under investigation. It is planned in the future to extend this study to the determination of activities in concentrated liquid metal solutions by use of Knudsen Cell techniques. The motivation for this study is to provide reliable information for the basic understanding of thermodynamic properties of liquid metal systems.

Transport Studies - Isothermal mass transfer across solid-liquid phase boundaries is being investigated in order to establish the rate controlling step and to test existing rate equations. Investigations in the systems zinc-mercury, tin-mercury and silver-mercury have indicated that existing rate laws are not obeyed under some conditions. A revised rate equation, assuming a variation of diffusion boundary layer with time, is being developed to treat these cases.

Recent Publications:

D. A. Stevenson, "The Solution Rate of Copper-Nickel Alloys in Lead," Trans. AIME, 221, (1961) p. 271.

Contractor: Stanford University, Stanford, California

Contract Number: AT(04-3)-298

Present Contract Term: May 1, 1962 through July 31, 1963

Cost to AEC: $54,581

Contract Title: KINETICS IN SOLID STATE SYSTEMS

Investigators: Victor F. Macres and Robert A. Huggins

Scope of Work:

A research program is presently being carried out which is aimed at obtaining a basic understanding of the mechanisms involved in certain diffusion controlled solid state reactions. Three distinct areas are being investigated which are related to the general problem of mass transfer by solid state diffusion at high solute contrations and over large composition ranges. Included in the experimental methods being employed are the techniques of electron microprobe and radioactive tracer analysis and nuclear magnetic resonance. The three areas include:

a. Ternary diffusion and its dependence on thermodynamic properties. The copper rich portion of the copper-cadmium-zinc system is being studied. Vapor-solid reactions are being used to obtain activity and diffusion behavior.

b. Effect of concurrent plastic deformation on solute diffusion. Studies of the zincification of copper and the dezincification of 60-40 brass have been made under concurrent tensile straining. Only slight effects were found and these results are being evaluated along with those published in the literature.

c. Diffusion studies in ordered ionic and covalent structures. Diffusion behavior of various cations in single crystal aluminum oxide and of solutes in 3-5 and 4-6 semiconducting compounds are being investigated. The influence of voltage gradients is being studied in some detail.

Recent Publications:

L. Neumann and R. A. Huggins, "Technique for Zone Melting of Insulators," Rev. Sci. Inst., April, 1962.

R. R. Dils, L. Zeitz, and R. A. Huggins, "A Suggested Secondary Fluorescence Correction Technique for Electron Probe Analyses in the Vicinity of a Steep Concentration Gradient," To be published in the Proceedings of the Third International Symposium on X-ray Microscopy and Microanalysis held at Stanford University, August, 1962.

Contractor:	Stanford University, Stanford, California
Contract Number:	AT(04-3)-326, Project # 2
Present Contract Term:	October 1, 1962 through September 30, 1963
Cost to AEC:	$20,000
Contract Title:	EFFECT OF LATTICE VACANCIES ON MECHANICAL BEHAVIOR OF CRYSTALLINE MATERIALS
Investigators:	Oleg D. Sherby

Scope of Work:

Phase transformation will cause iron to deform plastically when stressed uniaxially under small loads. Contrary to the results of other investigators it has been shown that the relation between phase transformation strain and stress is not linear. In addition, it has been shown that the alpha to gamma transformation contributes to a much larger transformation strain than the reverse polymorphic change gammato alpha. It is suggested that the origin of this weakening effect is associated with the generation of excess lattice vacancies created during the alpha to gamma transformation upon heating and the generation of excess interstitial atoms during cooling. The role of these excess point defects is to cause creep to take place since dislocation climb will be enhanced. In harmony with this suggestion it has been shown that the rate of heating and cooling plays an important role such that high rates of transformation lead to smaller transformation strains.

Recent Publications:

Oleg D. Sherby and Massoud T. Simnad, "Prediction of Atomic Mobility in Metallic Systems," Transactions, ASM, 54, (1961) pp. 227-240.

O. D. Sherby and M. T. Simnad, "Prediction of Atomic Mobility in Metallic Systems," (Discussions) Transactions, ASM, 54, (1961) pp. 771-779.

Contractor: Syracuse University, Syracuse, New York

Contract Number: AT(30-1)-1910

Present Contract Term: June 1, 1962 through May 31, 1963

Cost to AEC: $34,748

Contract Title: ALKALINE EARTH PHASE SYSTEMS

Investigators: F. Kanda and A. J. King

Scope of Work:

Several equilibrium systems are currently under investigation and near completion. These are the systems involving Sr-Mg, Sr-Na, Ba-Na, Ba-Mg, and Ca-Li. Intermediate phases are being investigated by single crystal Weissenberg techniques. It appears that all intermediate phases in the Ba-Mg and Sr-Mg systems are isomorphous whereas in the Ba-Li and Sr-Li systems they bear no resemblances to each other. It is hoped that crystallographic studies and high temperature calorimetry may indicate the reasons for the similarities and dissimilarities in these series of compounds. Calorimetric studies will also be utilized to investigate the retrograde melting phenomena in the Sr-Li system. Of interest in this investigation will be the thermodynamic data associated with the solid phase transition of Sr_8Li together with its ultimate retrograde melting and solidification into Sr_7Li.

Recent Publications:

F. E. Wang, F. A. Kanda, and Aden J. King, "The Crystal Structure of Sr_6Li_{23} and Sr_3Li_2," To be published.

F. E. Wang, F. A. Kanda and Aden J. King, "The Lithium-Strontium Equilibrium System," To be published.

Contractor:	Syracuse University, Syracuse, New York
Contract Number:	AT(30-1)-2731
Present Contract Term:	August 1, 1962 through July 31, 1963
Cost to AEC:	$19,941
Contract Title:	INVESTIGATION OF SPECIFIC VOLUMES OF LIQUID METALS AND ALLOYS
Investigators:	F. A. Kanda and D. V. Keller, Jr.

Scope of Work:

This is a study of the density of liquid melts as a function of temperature and composition. The purpose of the investigation is to attempt to uncover atomic volume dependent relationships similar to those described in the solid state. The apparatus incorporated for the high temperature density determinations by the displacement technique includes two automatic analytical balances, one of the mechanical, and the other of the electronic type which are capable of obtaining densities in the order of one part in 20,000. The change in apparent mass of the inert sinker is plotted automatically against the melt temperature as the melt temperature is decreased at a controlled rate. This technique, utilizing relative densities, was proposed originally for the identification of immiscibility boundaries in metal systems, i.e., Na-Li. A study now in progress involves an attempt to place these data on an absolute scale and finally the proof of Vegard's Law relationships in the liquid state. A second problem now under investigation involves the change in apparent atomic volume in the region of an intermetallic compound, Mg_2Sn, which has a high heat of formation. An analysis of these data with the heat capacity (Cp-Cv) data for this particular system may shed light on aggregations of compound units in the liquid state.

Contractor: Temple University, Philadelphia, Pennsylvania

Contract Number: AT(30-1)-2780

Present Contract Term: May 15, 1963 through May 14, 1964

Cost to AEC: $29,535

Contract Title: A SOLID STATE STUDY OF ZIRCONIUM AND NIOBIUM OXIDES

Investigators: Robert E. Salomon

Scope of Work:

The study of the photoeffects occurring with anodized zirconium and niobium electrodes will be continued. In particular, the high voltage photevoltaic effect that was found to occur at low temperatures will be investigated in great detail. These measurements will be extended to liquid helium temperatures. A determination of the complete spectral sensitivity of the short circuit photocurrent will be determined at low temperatures. The effect of oxygen and other gases on the normal photovoltaic effect will be studied. Improvements are being made in the apparatus to permit studies to be carried out are pressures below 10^{-7} mm.

Studies on the electronic and optical properties of bulk oxides that have been doped with various transition metal ion impurities will continue. Reflection spectra of solid solutions in fine powder form are made. The impurities have so far been incorporated by diffusion at 1200°C. We are planning to construct an electron beam furnace and mix the molten oxide with other transition metal oxides. The success of this method will depend on whether or not the added oxides are stable at the required temperature of 2800°C. X-ray diffraction measurements will be made on all samples to determine homogeneity and to detect possible phase changes.

Contractor: Temple University, Philadelphia, Pennsylvania

Contract Number: AT(30-1)-2812

Present Contract Term: August 1, 1962 through July 31, 1963

Cost to AEC: $49,469

Contract Title: STUDY OF THE IB-IIB BETA PHASE ALLOYS

Investigators: L. Muldawer and H. Amar

Scope of Work:

The general purpose of this study is the improvement of our understanding of alloys, in particular the beta-brass type alloys. The chief approaches include:

(1) Diffraction studies of structures and transformation. Ternary ordering has been shown to exist in $AgAuCd_2$, $AgAuZn_2$, and $AuCuZn_2$. The process of ternary ordering as a function of temperature is being investigated. A broader study of the possibility of disordering or considerable vacancy formation near melting is being considered.

(2) Spectral reflectivity as a function of composition, temperature and cold work. The effects of these variables upon optical properties is of interest. These studies, carried out in various alloy systems, should help in assigning the model to be used in interpreting optical properties. In order to make meaningful Kramers-Kronig calculations, it will be necessary to carry out reflectivity measurements over a wide range including vacuum ultraviolet.

(3) Theoretical studies and correlation with experimental results. An approximate calculation indicates that the main reflectivity edge of beta-brass in the visible is of plasma character. A detailed study to determine the specific roles of interband transitions and plasma effects is being undertaken. In order to obtain quantitative interpretation, a band structure calculation (using the Green's function method) is being planned.

Recent Publications:

F. Rothwarf and L. Muldawer, "Electrical Resistivity and X-Ray Diffraction Study of the Beta AgCd-AuCd System," J. of Appl. Phys. Vol 33, No. 8, (1962) pp. 2531-2538.

Contractor: Rensselaer Polytechnic Institute, Troy, New York

Contract Number: AT(30-1)-1044

Present Contract Term: December 1, 1962 through November 30, 1963

Cost to AEC: $45,038

Contract Title: ANISOTROPIC DIFFUSION AND ELECTROMIGRATION

Investigators: H. B. Huntington

Scope of Work:

This project has two principal lines of investigation.

In one of these we are concerned with diffusion in materials where the process is anisotropic. In the past we have investigated self-diffusion in zinc, cadmium, thallium and indium. Recent studies deal with impurities diffusion specifically in zinc. A marked dependence on solute valence is manifest. The diffusion of silver in zinc is approximately one order of magnitude slower than self-diffusion, that of indium one order of magnitude faster. In the latter case the sign of the anisotropy is reversed. These results have been shown to be in fair quantitative agreement with the predictions of a shielded ion model. Work on diffusion of antimony and cadmium in zinc is under way.

The other line of investigation concerns atom movements as affected by high electric currents. In the past we have observed current-induced marker motion in gold and copper wires and are at present studying platinum and aluminum. With the gold and copper the direction of mass motion at low temperature indicates the influence of the pressure of the charge carriers on the moving atoms. With the platinum wires the effects of thermal gradient and surface forces also are clearly evident. Future plans call for investigating a large number of pure metals, several with lower melting points. To determine temperature accurately without pyrometry will require cylindrical shells large enough to insert a moveable thermocouple inside. For the larger currents required a 1500 amp dc supply has been constructed and tested with aluminum specimens.

Recent Publications:

H. B. Huntington and A. R. Crone, "Current-induced Marker Motion n Gold Wires," J. Phys. Chem. Solids 20, (1961) p. 76.

A. R. Crone, "Current-induced Marker Motion in Copper," J. Phys. Chem Solids 20, (1961) p. 88.

J. H. Rosolowski, "Diffusion of Silver and Indium in Zinc," Phys. Rev., 124, (1961) p. 1829.

T. H. Hehenkamp, "A Sensitive Optical Pyrometer," J. Sci. Instr., 33, (1962) p. 229.

H. B. Huntington and P. B. Ghate, "A New Method for Treating Vacancy Correlation," Phys. Rev. Letters, 8, (1962) p. 421.

P. B. Ghate and H. B. Huntington, "Diffusion of Cadmium (115m) in Zinc," Bull. APS II, 7, (1962).

Contractor: Rensselaer Polytechnic Institute, Troy, New York

Contract Number: AT(30-1)-1995

Present Contract Term: February 1, 1963 through January 31, 1964

Cost to AEC: $37,165

Contract Title: THEORETICAL RESEARCH RELATING TO RADIATION DAMAGE IN SOLIDS

Investigators: Edmond Brown

Scope of Work:

Theoretical studies of energies and configurations of point defects in copper will be continued. In particular, an electron energy band method will be used to study the contribution of conduction band electrons to the energy. This method will utilize a model in which a periodic array of defects is placed in the crystal. These will be placed sufficiently far apart to be approximately isolated but near enough so that the unit cell has a reasonable number of atoms. With the development of recent theoretical approaches to the band structure problem this approach should be tractable with use of a high speed computer.

In addition to the study of isolated defects some work has begun on close interstitial-vacancy pairs and on di-interstitials. This work will be extended.

Some preliminary work may be carried out on silver and gold. These metals require an extension of the present model, as the elastic constants cannot be fit well using nearest neighbor central forces.

Recent Publications:

R. A. Johnson and E. Brown, "Point Defects in Copper," Physical Rev., Vol. 127, No. 2, (1962) pp. 446-454.

G. H. Goedecke and E. Brown, "Variational Principle for Potential Scattering," Physical Rev, Vol 125, No 6, (1962) pp. 2116-2124.

Contractor: Rensselaer Polytechnic Institute, Troy, New York

Contract Number: AT(30-1)-2159

Present Contract Term: May 1, 1962 through April 30, 1963

Cost to AEC: $38,940

Contract Title: MECHANISM OF THE EFFECT OF RARE EARTH SOLUTES ON THE ALLOTROPIC TEMPERATURE OF ZIRCONIUM

Investigators: A. A. Burr

Scope of Work:

Following the development of a suitable method for the production of zirconium-rare earth alloys, preliminary investigations of the effect of rare-earth solutes on the allotropic transformation temperature of zirconium were undertaken employing the following techniques: resistivity measurements, dilatometry, and metallography.

It was found that Nd had a lowering effect on the resistivity of Zr; this peculiar behavior requires further study. From the dilatometric results, Q_b values were calculated for the Zr-Yt, Zr-Dy, Zr-Ho, and Zr-Er systems. In addition, these dilatometric results, coupled with the results of the resistivity measurements, provided a basis for metallographic determination of the partial phase diagrams for the above zirconium-rare earth systems. Suitable techniques in metallography have been developed for this purpose.

It is evident from these studies that: (1) due to the presence of impurities which are difficult to avoid, these alloy systems cannot be regarded as simple binaries, and (2) the alpha region is stabilized by the rare-earth solutes. Furthermore, the large differences in solubilities indicated a deviation from basic alloy theory. It therefore becomes pertinent to investigate the role of electron configuration in alloying while data from the above studies are being refined and enlarged to cover the Zr-Gd, Zr-Tb, Zr-Tm, and Zr-Lu systems. Future work will also include heat-capacity measurements as another method for the study of alloying behavior.

Contractor:	Rensselaer Polytechnic Institute, Troy, New York
Contract Number:	AT(30-1)-2408
Present Contract Term:	June 1, 1962 through May 31, 196
Cost to AEC:	$22,008
Contract Title:	MECHANISM OF SINTERING LOOSE AND PRESSED METAL POWDER COMPACTS
Investigators:	F. V. Lenel

Scope of Work:

This project is concerned with the driving force and the material transport mechanisms which occur during sintering of a single metal powder either in the form of loose powder or of a pressed compact. In a first investigation it was shown that gravity forces in addition to surface tension forces contribute to the dimensional changes in sintering of copper powder compacts in the temperature range near 900°C. This fact was established by comparing the radial shrinkage near the top of compact with that near the bottom of compacts.

In a second investigation the mechanism of material transport in a loose powder aggregate of spherical silver powder at temperatures near 300°C was determined by measuring the changes in electrical resistance of the aggregate with time at several temperatures, relating these changes to changes in contact area, and determining the activation energy of the contact area growth process. The activation energy changes as a function of applied stress in a manner identical to changes in activation energy with stress during creep testing of silver in this temperature range. A transport mechanism of plastic deformation due to cross slip is postulated.

A third investigation concerns the role of plastic deformation by dislocation climb as a material transport mechanism in sintering. To throw light on this problem experiments are conducted in which the dimensional changes of compacts are determined dilatometrically as a function of applied exterior stress and in which the changes in electrical conductivity with time of spherical particle models are being measured.

Recent Publications:

F. V. Lenel, H. H. Hausner, E. Hayashi and G. S. Ansell, "Some Observations on the Shrinkage Behavior of Copper Compacts and of Loose Powder Aggregates," Powder Metallurgy, No. 8, (1961) p. 25.

F. V. Lenel, H. H. Hausner, I. A. El Shanshoury, J. G. Early and G. S. Ansell, "The Driving Force for Shrinkage in Copper Powder Compacts during the Early Stages of Sintering," Accepted by Powder Metallurgy.

F. V. Lenel, H. H. Hausner, O. V. Roman and G. S. Ansell, "The Influence of Gravity upon the Shrinkage of Copper Powder Compacts," Accepted by Acta. Met.

Contractor: Rensselaer Polytechnic Institute, Troy, New York

Contract Number: AT(30-1)-2714

Present Contract Term: February 1, 1963 through January 31, 1964

Cost to AEC: $27,064

Contract Title: THE ELECTROCHEMICAL AND CORROSION CHARACTERISTICS OF RARE EARTH AND YTTRIUM METALS

Investigators: N. D. Greene

Scope of Work:

Corrosion Behavior of the Rare Earth Metals

Oxidation tests in dry and moist air at low and high temperatures to study the kinetics of oxide film formation. These data will be compared to the results of aqueous corrosion tests to determine the relative influence of solid state electronic structure and the kinetics of film formation on corrosion rates.

Electrochemical Characteristics of the Rare Earth Metals

Anodic polarization studies in phosphoric acid solutions above 0.1 normal. Measurements will also be conducted in other media such as sodium and ammonium hydroxide and buffered acid solutions.

Hydrogen overvoltage studies in phosphoric acid and sodium hydroxide. The current aim is to find a suitable electrolyte for all the metals to permit direct comparison of overvoltage parameters.

Dissolution of Uranium, Thorium, and Their Alloys

Dissolution behavior of thorium in sulfuric and other acids: Studies of the transpassive behaviors of uranium and thorium to determine optimum dissolution conditions.

Contractor:	Rensselaer Polytechnic Institute, Troy, New York
Contract Number:	AT(30-1)-3004
Present Contract Term:	April 1, 1963 through March 31, 1964
Cost to AEC:	$22,595
Contract Title:	DENDRITE GROWTH IN SUPERCOOLED METALS
Investigators:	Wylie J. Childs

Scope of Work:

The mechanism of dendrite growth has received increasing attention in recent years. This study has been undertaken to study the two principal factors in dendrite growth.

The first of these factors is the effect of the amount of supercooling on the velocity of dendrite growth for pure metals of different crystal systems. Velocity measurements are being made employing a .003 inch diameter three junction thermoelectric transducer coated with a silicone compound to act as an insulating agent. This transducer, originally developed by Glicksman, measures the movement of the thermal wave associated with recalescence as growth progresses through the freezing liquid. The temperature gradients within the cooling liquid metal are also being measured to study the reason for rapid growth of surface dendrites.

The dendrite growth rate is also being studied for alloys in order to study the influence of solute atoms on the mechanism of growth. It has been postulated that heat transport is the limiting factor in growth of supercooled pure metals. This postulation is being studied as well as the influence of solute atom movement in alloys during dendrite freezing.

The second aspect of the program deals with dendrite shape. Current theoretical analysis of dendrite growth are limited because little is known about the morphology of dendrites. Dendrite morphology will be studied as a function of supercooling for pure metals and alloy systems employing vacuum decanting and X-ray techniques.

Contractor: Rensselaer Polytechnic Institute, Troy, New York

Contract Number: AT(30-1)-3030

Present Contract Term: May 1, 1962 through July 31, 1963

Cost to AEC: $22,000

Contract Title: NUCLEAR QUADRUPOLE COUPLING STUDIES IN SOLIDS

Investigators: Philip A. Casabella

Scope of Work:

The proposed studies fall into four groups:

1. The Group III Halides - Earlier work by Professor Casabella has shown the fruitfulness of the study of nuclear quadrupole coupling constant in these compounds. Considerable information has been obtained concerning their crystalline and molecular structure. Several of these compounds have not yet been studied by this method, but will be under this contract.

2. Ferroelectrics - Nuclear quadrupole coupling will be studied in ferroelectric crystals. The studies will be made as a function of temperature in order to observe the changes that take place at the ferroelectric transition temperatures. This work will begin with the study of the nuclear quadrupole coupling of sodium in Rochelle salt.

3. Effects of Co^{60} Radiation - Irradiations by Co^{60}-rays cause a marked decrease in the intensities of pure quadrupole resonances. In some crystals the effect lasts only a few hours, while in others it seems permanent. More work will be done in an effort to find the causes of these effects.

4. Nuclear Quadrupole Coupling of Nitrogen - This is of interest since N^{14} is the only nucleus with a spin of one which occurs in abundance in nature. The resulting data is particularly easy to analyze, and there is still work to be done on the effect of a weak magnetic field on a N^{14} pure quadrupole resonance.

Contractor: National Bureau of Standards, Washington, D.C.

Contract Number: NBS Project No. 13443

Present Contract Term: July 1, 1962 through June 30, 1963 (Fiscal Year 1963)

Cost to AEC: $20,000

Contract Title: DIELECTRIC PROPERTIES OF CRYSTALS

Investigators: H. P. R. Frederikse and J. H. Wasilik

Scope of Work:

The general objective of this program is to study the dielectric constant and losses of pure inorganic crystals and crystals containing imperfections.

From an analysis of the barrier layer at the electroded surface of a piezoelectric semiconductor, it has been shown under what conditions the piezoelectric coefficient of a material can be determined from measurements at the acoustic resonance of the sample.

Considerable attention is being given to the observation of dielectric effects connected with excitations in CdS since the exciton has a large polarization leading one to expect it to contribute significantly to the real part of the dielectric constant.

Other materials being studied are pure and doped PbF_2, LiF doped with Ti or V, and $SrTiO_3$.

Contractor: Nebraska, University of, Lincoln, Nebraska

Contract Number: AT(11-1)-525

Present Contract Term: June 1, 1962 through May 31, 1963

Cost to AEC: $35,480

Contract Title: STUDIES OF IMPERFECTIONS IN SOLIDS

Investigators: Edgar A. Pearlstein

Scope of Work:

Experimental work is being done on: (1) Radiation effects in metals, (2) Stored energy in x-rayed alkali halide crystals, (3) Mechanisms of color center production in alkali halide cyystals, and (4) Thermal production of vacancies in sodium metal.

(1) Copper foils are irradiated at liquid nitrogen temperature with protons of energy 50 to 350 keV, and changes of electrical resistivity measured. It is planned to use also helium ion irradiation. The purpose of the work is to check the dependence of radiation effects upon the energy and mass of the bombarding particles. Surface effects are also being looked for by irradiating at oblique incidence.

(2) Crystals are irradiated by x-rays at liquid nitrogen temperature. The heat given off as they are warmed to 400°C is measured and correlated with changes in optical absorption.

(3) a) It was found that, in some speciments of KCl and NaCl, simultaneous irradiation with x-rays and light predisposes the crystals to color faster, on subsequent irradiation with x-rays in the dark, than if they has originally been irradiated in the dark. The effect is being investigated further, to see if it means that there is a transient stage in the production of F-centers. b) Thin platelets of NaCl can be grown from solution with very few dislocations, as determined by an x-ray technique. The ease of F-center production in these crystals is being correlated with the dislocation content.

(4) Measurements of length and of x-ray lattice parameter are made simultaneously on single crystals of sodium metal, at temperatures from -50 to +97°C. Differences in the two temperature coefficients are interpreted in terms of the thermal production of vacancies.

Recent Publications:

E. A. Pearlstein, "New Bridge Circuit for Comparing Four Terminal Resistors," The Review of Scientific Instruments, Vol. 33, No. 6, (1962) pp. 610-612.

Fred T. Phelps, Jr. and E. A. Pearlstein, "Measurement of the Stored Energy in X-Rayed Sodium Chloride," Physical Review, Vol. 128, No. 4, (1962) pp. 1575-1585.

Contractor: New York University, University Heights, New York

Contract Number: AT(30-1)-2916

Present Contract Term: January 1, 1963 through December 31, 1963

Cost to AEC: $26,459

Contract Title: THERMODYNAMIC PROPERTIES OF INTERMETALLIC COMPOUNDS

Investigators: Kurt L. Komarek

Scope of Work:

The shape of the liquidus near an intermediate compound and the heat of fusion are being used quantitatively to evaluate the relative thermodynamic functions near the melting points of intermediate compounds of a selected group of binary systems: AB_2 compounds of magnesium with elements of group IV i.e. compounds with Si, Ge, Sn, Pb.

The melting points and the liquidus near the compounds are being determined by precision thermal analysis, and the heat of fusion of Mg_2Si will be obtained by a special calorimetric method. The extent of solid solubility of the compound is being determined by solidifying samples by the Bridgman method at different liquidus temperatures and analyzing the portion first solidified both chemically and by x-rays. Should the compound have a very small range of solid solubility the electrical resistivity of these samples will be used to determine solubility limits and any deviation of the maximum melting point from the stoichiometric compostion.

The results for the liquidus curves are being correlated to measurements of electrical resistivity in the liquid above the melting point. The data will be evaluated with special emphasis on the temperature range close to the melting point. The deflection in the plot of the chemical potential vs. mole fraction is being determined and compared with the resistivity measurements in the liquid.

In addition, work has just been started on a study of retrograde melting of intermetallic compounds.

Contractor:	North Carolina, University of, Chapel Hill, North Carolina
Contract Number:	AT(40-1)-2036
Present Contract Term:	April 1, 1962 through March 31, 1963
Cost to AEC:	$15,742
Contract Title:	RESEARCH IN INTERMETALLIC DIFFUSION
Investigators:	Lawrence Slifkin

Scope of Work:

The study of the effects of a vacancy flux on tracer diffusion will be continued. The Ag-Au system is being employed; it is one in which the two constituents have sufficiently different diffusion coefficients to produce an appreciable Kirkendall effect and yet over a rather large composition range the tracer D's are independent of composition. Thus, the tracer will see a vacancy flux but not a gradient in D. Also to continue are tracer diffusion measurements in alpha phase silver-based alloys, in conjunction with Zener relaxation studies at Wake Forest College. The aim here is to explore the generality of preliminary indications that the activation energy of the Zener peak is the same as that of the diffusion of the fast tracer. Preliminary experiments on Cu-17%Al suggests that the activation energy for Cu* diffusion is the same as in pure copper. More extensive measurements on an alloy of slightly lower Al content will be performed to verify this early result. To be initiated are tracer diffusion experiments on ordering binary alloys, one to investigate the possible effects on the dynamic ordering process itself in accelerating diffusion, and the other to explore the effects of order in alloys of the type A_3B where each B-site is surrounded by A-sites but not vice versa. Experiments on point defects in silver chloride will continue. We have found that it is possible to quench in excess vacancies in AgCl, and future work will be along the line of exploring X-irradiation effects on the color and ionic conductivity of such crystals and a search for a dielectric relaxation and increase in dielectric constant due to vacancy pairs.

Recent Publications:

W. C. Mallard, A. B. Gardner, Ralph F. Bass and L. M. Slifkin, "Self-Diffusion in Silver-Gold Solid Solutions," Submitted to The Physical Review.

H. P. Layer and R. O. Meyer, "Improved Precision Chuch for Sectioning Diffusion Samples," Submitted to Review of Scientific Instruments.

G. P. Williams, Jr. and L. M. Slifkin, "Tracer Insolubility and the Anomalous Diffusion of Rare Earths in Silver and Lead," Submitted to Acta Met.

H. P. Layer and L. M. Slifkin, "Studies of Point Defects in AgCl," Accepted by Journal of Physical Chemistry.

Contractor: North Carolina, University of, Chapel Hill, North Carolina

Contract Number: AT(40-1)-2577

Present Contract Term: June 1, 1962 through May 31, 1963

Cost to AEC: $31,547

Contract Title: RADIATION DAMAGE AND OTHER STUDIES BY MEANS OF A VAN DE GRAAFF ACCELERATOR

Investigators: Paul E. Shearin

Scope of Work:

Radiation damage studies in copper, aluminum and alloys of aluminum are underway. Damage is introduced through electron bombardment at temperatures near 12°K and also near 80°K. Damage is measured by measuring the change in electrical resistance. The recovery of damage is studied through isochronal anneals for the temperature range 16°K to 400°K. Particular attention is given to multiple defect production.

A simple cryostat for bombardment near liquid nitrogen temperature has been constructed. Special techniques have been developed for accurately controlling the temperature at which liquid nitrogen boils by controlling the pressure. This permits bombardment and subsequent isochronal anneals based on resistance measurements at this standardized temperature. Without some such control the boiling temperature of nitrogen varies too much with variations in impurity content and in atmospheric pressure to permit this to be used as a reference temperature.

Recent Publications:

Robert L. Chaplin and Paul E. Shearin, "Energy-Dependent Behavior of Intrinsic Class-Pair Defects within Copper," Phys. Rev. 124, (1961) p. 1061.

R. L. Chaplin and P. E. Shearin, "Some Experimental Techniques of Low-Temperature Radiation Damage Studies," Accepted by Review of Scientific Instruments.

Contractor: North Dakota, University of, Grand Forks, North Dakota

Contract Number: AT(11-1)-1255

Present Contract Term: June 1, 1963 through May 31, 1964

Cost to AEC: $9,028

Contract Title: RADIATION DAMAGE TO SILICA STRUCTURES

Investigators: Harold D. Bale

Scope of Work:

Radiation induced changes in silica structures will be studied by x-ray diffraction methods. Silica gels and vitreous silica will both be studied but primary emphasis will be placed on the study of the gels. Silica gels are often characterized by their specific surface which can be as high as 600 m^2/gm. Small angle x-ray scattering is one of the most sensitive means of studying variations in the specific surface of a substance. Plans are to carefully observe the small angle scattering from the gels before and after irradiation. Attempts will be made to relate changes in the scattering to changes in specific surface area and also changes in the average size parameter of the gel inhomogeneities.

Other workers have estimated that a single damaged region in vitreous silica may contain about 10^3 to 10^4 atoms. Regions of this size would be well suited for study by small angle scattering and it is hoped that a small angle scattering study of damaged vitreous silica will yield more direct information about the size of these damaged regions. If the damaged regions have a characteristic shape this could probably also be determined from the shape of the scattering curve.

Large angle scattering will also be measured from the gel samples and from the data radial distribution curves will be obtained. Similar large angle studies of vitreous silica have been made previous by other workers.

Pile irradiation of about 10^{19} to 10^{20} fast neutrons/cm^2 will be used to damage the structures. Effects of prolonged gamma irradiation will also be investigated.

Contractor: Northwestern University, Evanston, Illinois

Contract Number: AT(11-1)-1126

Present Contract Term: February 1, 1963 through January 31, 1964

Cost to AEC: $10,221

Contract Title: CONTRIBUTION TO THE UNDERSTANDING OF THE HIGH TEMPERATURE OXIDATION OF METALS

Investigators: J. Bruce Wagner, Jr.

Scope of Work:

Oxidation studies have been initiated on zone-refined iron doped with very small amounts of chromium. In $CO-CO_2$ mixtures the rate is linear with time in analogy with data for pure iron (F. Pettit, R. Yinger and J. B. Wagner, Jr., Acta Met. 8, (1960) p. 617). The transition from linear to parabolic kinetics is being studied as a function of temperature, pressure, and electron hole concentration in the wüstite layer.

Electrical conductivity studies are being carried out on pure wüstite and chromium-doped wustite as a function of temperature and oxygen partial pressure. Similar measurements are being carried out on natural single crystals of hematite and on sintered powders of Fe_2O_3.

Contractor: Northwestern University, Evanston, Illinois

Contract Number: AT(11-1)-1161

Present Contract Term: April 1, 1963 through March 31, 1964

Cost to AEC: $38,000

Contract Title: STUDY OF RADIATION DAMAGE RESULTING FROM ELECTRON BOMBARDMENT

Investigators: John W. Kauffman

Scope of Work:

The purpose of this work is the study of the fundamental nature of the changes produced in crystalline materials as the result of electron irradiation, and the interrelation of these fundamental structural changes with physical properties. The present studies are on metals and alloys and initial preliminary studies are beginning on semiconductors.

The irradiation used in these studies is a mono-energetic electron beam from a Van de Graaff generator. The energies used are from 0.1 Mev up to a maximum energy close to 5 Mev. The present cryostats allow irradiations and subsequent studies to be carried out near liquid helium temperatures and above. An IBM 709 computer is used in the analysis of various aspects of this research. In the past year further studies have been carried out on pure gold and other additional pure metals as well as several alloys.

Recent Publications:

J. B. Ward and J. W. Kauffman, "Low-Temperature Recovery of Resistivity in Electron-Irradiated Gold," Physical Review, Vol. 123, No. 1, (July, 1961) pp. 90-96.

Contractor:	Oklahoma, University of, Norman, Oklahoma
Contract Number:	AT(40-1)-2570
Present Contract Term:	May 1, 1962 through April 30, 1963
Cost to AEC:	$13,895
Contract Title:	AN INVESTIGATION OF THE INFLUENCE OF HYDROGEN ON MECHANICAL PROPERTIES OF METALS. PHASE I: HYDROGEN IN NIOBIUM
Investigators:	Raymond D. Daniels

Scope of Work:

The segregation of hydrogen to incipient microcrack vertices during plastic straining is believed to be a cause of low temperature brittle fracture in hydrogenated columbium. A program at the University of Oklahoma has been concerned with the problem of brittle fracture of metals as affected by interstitial elements such as hydrogen. The fracture behavior of columbium containing amounts of hydrogen at or below the limit of solubility has been studied. Hydrogen embrittles columbium even at concentrations below the limit of solubility. The concentration necessary to effect a given degree of embrittlement increases with increasing temperature. However, the behavior of hydrogen in columbium is unusual, as compared to other interstitial contaminate elements, in that, at very low temperatures (minus 321 degrees Fahrenheit) a restoration of ductility is observed. The minimum in ductility occurs at the temperature where the reduced mobility of hydrogen begins to limit hydrogen redistribution during the tensile test.

Contractor:	Pennsylvania State University, University Park, Pennsylvania
Contract Number:	AT(30-1)-1710
Present Contract Term:	April 1, 1963 through March 31, 1964
Cost to AEC:	$52,386
Contract Title:	RESEARCH ON GRAPHITE
Investigators:	P. L. Walker, Jr. and H. B. Palmer

Scope of Work:

The formation kinetics, properties, and reactions of pyrolytic carbon films are being studied. The two approaches used in this work are (a) to make direct measurements of film growth rates in a flow system and (b) to measure gas-phase decompostion kinetics, also in flow systems. Fairly detailed studies of formation kinetics have been carried out for film formed by pyrolysis of methane and carbon suboxide, while preliminary work has been done using benzene and toluene. A study of gas-phase pyrolysis of acetylene has been completed, the results of which will be used in an attempt to form a complete phenomenological description of carbon film formation from benzene. Further work on the properties and gasification of carbon films is planned, as well as an extension of the film formation kinetics studies.

The study of the kinetics and mechanism of the reaction of carbon with oxidizing gases is continuing. It is divided into five phases: one, the mechanism by which impurities catalyze the reaction of graphite with oxidizing gases; two, the effect of impurity additives on the solid state properties of graphite (electrical conductivity, magnetic susceptibility, and thermoelectric power); three, determination of the individual rate constants in the spectroscopic graphite-carbon dioxide reaction as a function of temperature and burn-off; four, the effect of gas and pore size on the steady-state counter-diffusion of gases in graphite; and five, light microscope studies on the oxidation of graphites of large crystalline size.

Recent Publications:

F. J. Vastola and P. L. Walker, Jr., "The Reaction of Graphite 'Wear Dust' with Carbon Dioxide and Oxygen at Low Pressures," J. Chem. Phys., 58, (1961) p. 20.

B. C. Banerjee and P. L. Walker, Jr,, "Electrolytic Micromachining of Iron Whisker Surfaces," J. Electrochem. Soc. 108, (1961) p. 262.

B. C. Banerjee and P. L. Walker, Jr., "On the Mechanism of Cathodic Crystal Growth Processes," J. Electrochem. Soc. 108, (1961) p. 449.

B. C. Banerjee and P. L. Walker, Jr., "Interaction of Evaporated Carbon Films with Nickel," J. Appl. Phys., in press.

T. J. Hirt and H. B. Palmer, "Carbon Films from Carbon Suboxide Decomposition. I. Formation Kinetics," Proceedings of the Fifth Biennial Carbon Conference, Pergamon Press, New York, in press.

B. C. Banerjee, T. J. Hirt, and P. L. Walker, Jr., "Pyrolytic Carbon Formation from Carbon Suboxide," Nature, in press.

B. C. Banerjee and P. L. Walker, Jr., "Electron Microscopic Investigation on Structure and Topography of Electrodeposited Nickel," J. Electrochem. Soc., in press.

R. S. Slysh and C. R. Kinney, "Some Kinetics of the Carbonization of Benzene, Acetylene and Diacetylene at 1200°," J. Phys. Chem. 65, (1961) p. 1044.

J. F. Rakszawski, F. Rusinko, Jr., and P. L. Walker, Jr., "Catalysis of the Carbon-Carbon Dioxide Reaction by Iron," Proceedings of the Fifth Biennial Carbon Conference, Pergamon Press, New York, in press.

P. L. Walker, Jr. and W. V. Kotlensky, "Apparent Densities and Internal Surface Areas of Selected Carbon Blacks," Can. J. Chem., in press.

P. L. Walker, Jr., "Carbon---An Old But New Material," American Scientist, in press.

Contractor:	Pennsylvania State University, University Park, Pennsylvania
Contract Number:	AT(30-1)-1858
Present Contract Term:	October 1, 1962 through September 30, 19 3
Cost to AEC:	$52,800
Contract Title:	EFFECT OF RADIATION ON DYNAMIC PROPERTIES OF HIGH POLYMERS
Investigators:	J. A. Sauer

Scope of Work:

The studies being carried out include radiation studies of some specific high polymers, studies of transitions and molecular motion in polymers with emphasis on low temperature behavior, and wave propagation studies of solids of various shapes and also composite systems. One of the contemplated radiation studies is to investigate more fully the effect of pile irradiation on teflon kept in an oxygen-free atmosphere. The molecular motion studies include both proton magnetic resonance investigations and dynamic mechanical investigations in the temperature range from $4^{o}K$ to $80^{o}K$, deuteron resonance studies from $80^{o}K$, and thermal expansion studies from $80^{o}K$, dielectric studies of various co-polymers in solution, and thermal conductivity studies of several polymers at temperatures encompassing transition regions. Efforts will be devoted to studying the mechanism of crystallization of polypropylene single crystals and to producing large crystals of definite fold period for investigation by NMR and mechanical methods. Wave propagation studies will include both theoretical analysis of complex systems as well as of single specimen shapes and experimental investigations to extend the frequency range of measurements and to provide accurate measure of mechanical properties of very small specimens.

Recent Publications:

E. J. Skudrsyk, B. R. Kautz and D. C. Greene, "Vibration of, and Bending-Wave Propagation in Plates, " J. Acoust. Soc. Am. 33, (1961) p. 36.

A. E. Woodward, J. A. Sauer, and R. A. Wall, "Dynamic Mechanical Behavior of Some Partially Crystalline Poly-Olefins," J. Polymer Science 50, (1961) p. 117.

A. E. Woodward, J. A. Sawer and A. Odajima, "Proton Magnetic Resonance of Some Poly- -Olefins and -Olefin Monomers," Accepted by J. Physical Chemistry.

A. Odajima, A. E. Woodward and J. A. Sauer, "Proton Magnetic Resonance of Some -Methyl Group Containing Polymers and Their Monomers," Accepted by J. of Polymer Science.

M. N. Stein, R. G. Lauttman, J. A. Sauer and A. E. Woodward, "Dielectric Loss in Poly(Hexamethylene Adipamide) and Poly(Hexamethylene Sebacamide) at Low Temperatures," Accepted by J. Applied Physics.

A. Jacobs and D. E. Kline, "Energy Deposition in Polymers by Reactor Radiation," Accepted by J. Applied Polymer Science.

D. E. Kline, "Thermal Conductivity Studies of Polymers," Accepted by J. Polymer Science.

D. E. Kline, "Radiation Effects in Polystyrene," Accepted by J. Polymer Sceince.

Contractor:	Pennsylvania State University, University Park, Pennsylvania
Contract Number:	AT(30-1)-2541
Present Contract Term:	April 1, 1963 through March 31, 1964
Cost to AEC:	$28,391
Contract Title:	HIGH TEMPERATURE PROPERTIES OF TITANIUM AND ZIRCONIUM PHOSPHIDES AND RELATED REFRACTORY MATERIALS
Investigators:	Karl Gingerich

Scope of Work:

The purpose of the present research is to continue the investigation of high temperature properties of transition metal phosphides with emphasis on thos of group IV.

A mass spectrometric survey study of the vaporization of selected monophosphides of actinides, lanthanides and group IV - Vi transition metals has established the relative thermal stabilities and the vaporization behavior. The most stable phosphides are those formed by the actinides, then follow in decreasing order the phosphides of the lanthanides, group IV, group V, and group VI transition metals. Within group IV there is a marked increase in stability with atomic number. Only UP vaporizes congruently. All other phosphides studied vaporize by decompostion into phosphorus and a condensed phase of lower phosphorus content. The thermal expansion of the monophosphides of Ti, Zr, and Hf has been measured by x-ray diffraction. The compositional and temperature transformation for α-ZrP $\rightleftarrows$ β-ZrP has been studied and explained by a model. The rate of phosphidation of zirconium at 1000°C has been found to be linear for reaction layers less than 0.05 mm thick.

The mass spectrometric studies are being continued for more metal rich phases. Phosphorus dissociation pressures are to be measured by static methods, using Bourdon gauge and radio tracer techniques. Further x-ray investigations will be undertaken to determine existent phases and their homogeneity ranges. Thermal analysis will be used for melting point determinations.

Contractor:	Pennsylvania State University, University Park, Pennsylvania
Contract Number:	AT(30-1)-2581
Present Contract Term:	June 1, 1963 through May 31, 1964
Cost to AEC:	$112,575
Contract Title:	FUNDAMENTAL STUDIES IN HIGH TEMPERATURE MATERIALS PHENOMENA
Investigators:	M. E. Bell

Scope of Work:

(1) In the dielectrics area, a highly sensitive equipment for the new noncontract rotating field method of dielectric measurement has been designed and constructed. For the soda-alumina-silica glass system, new data have been obtained on the electrical conductivity at very high pressures. Pyroelectric measurements on Bi-Sr titanate single crystals have shown that the massive dielectric relaxation in these specimens is associated with the onset of ferroelectricity.

(2) The resistivity data on powdered material indicates clearly the importance of the surface state and contact between particles. With powder junctions, it is possible in the Cr_2O_3-ZnO system to determine the onset of the reaction by electrical measurements.

(3) The work on the titanium-oxygen system has produced the first clear evidence of the position of the Magneli phases in the oxygen pressure-temperature diagram.

(4) A wide-ranging survey has shown that infrared spectra may be used as a tool to determine the coordination of the metal ion in simple oxide structures.

(5) Development of the modified hot wire method for measuring thermal conductivity has been completed. A program is being initiated to exploit the extreme simplicity of this method to make measurements at high temperatures and pressures.

Contractor:	Pennsylvania State University, University Park, Pennsylvania
Contract Number:	AT(30-1)-2781
Present Contract Term:	May 1, 1963 through April 30, 1964
Cost to AEC:	$15,875
Contract Title:	THERMODYNAMICS OF SOLID SOLUTIONS AT HIGH TEMPERATURES
Investigators:	Arnulf Muan

Scope of Work:

Equilibria among the cobalt oxides themselves as well as thermodynamic properties of solid solutions with periclase type structure have been determined during the first term of the contract. These solid solutions have been shown to be either ideal or to have a slight positive deviation from ideality. Approximate phase relations have also been delineated in cobalt oxide containing systems where spinel, olivine and pyroxene solid solutions are present. Results of the latter studies have set the stage for an attack on thermodynamic properties of these more complex phases. Preliminary activity measurements in iron-cobalt spinels have indicated a very pronounced deviation from ideal behavior. Continuation and expansion of the work on the thermodynamics of spinels and initiation of similar work on olivine and pyroxene solid solutions are the main objectives of the research proposed for next year. Our experimental methods have now been developed to the point where it will become possible and desirable to study solid solution phases in which iron oxide is a component in addition to or instead of cobalt oxide.

Contractor:	Pennsylvania State University, University Park Pennsylvania
Contract Number:	AT(30-1)-2792
Present Contract Term:	June 1, 1962 through May 31, 1963
Cost to AEC:	$29,336
Contract Title:	THE MECHANISMS OF FISSION GAS DIFFUSION IN GRAPHITE
Investigators:	W. S. Diethorn and P. L. Walker, Jr.

Scope of Work:

The objective of the program is to investigate the effect of graphite structure and temperature on the diffusion of fission gas through fueled graphite. The program consists of three phases in the order listed below.

Phase 1

Postirradiation fission-gas diffusion studies with natural graphite powder and cold-pressed fueled bodies of this material up to temperatures of 2500F. Once mechanisms of fission gas release are established from these out-of-pile fission-gas diffusion studies in Phase 2.

Phase 2

Low-flux, in-pile fission gas diffusion studies of fueled bodies made with materials studied in Phase 1. These studies will be carried out over a range of temperatures, the upper limit approaching 2000F. A small number of experiments is planned for this phase of the program.

Phase 3

Postirradiation and in-pile fission gas diffusion studies of fueled artificial graphite. This phase of the program will be limited to a few carefully selected reactor-grade graphites of major interest to graphite vendors and reactor designers.

Contractor:	Pennsylvania State University, University Park, Pennsylvania
Contract Number:	AT(30-1)-2887
Present Contract Term:	October 1, 1962 through September 30, 1963
Cost to AEC:	$15,666
Contract Title:	PREPARATION, PROPERTIES, AND STRUCTURE OF CARBONATE GLASSES
Investigators:	O. F. Tuttle

Scope of Work:

The principal objective of this research is to investigate the pressure-temperature range over which carbonate and related glasses can be produced, and to measure certain physical and chemical properties of the glasses. Glasses were found to form readily in the system K_2CO_3-$MgCO_3$ in the 40, 50 and 60 mole percent mixtures. In mixtures containing mre than ~60 or less than ~40 mole percent $MgCO_3$ the liquids devitrified on cooling. The system is of the simple eutectic type and is characterized by a eutectic at 42 mole percent $MgCO_3$ at 440°C and 15,000 psi. Compositions containing more than ~70 mole percent $MgCO_3$ dissociated to MgO - liquid - vapor at 15,000 psi. At temperatures below 300°C at low pressure, the compound $K_2Mg(CO_3)_2$ becomes stable.

Glasses having the composition 55 CaO, 10 MnO, 25 CO_2, 10 H_2O (wt. percent) were also prepared at 15,000 psi. at temperatures from 900°C to 1,200°C. These liquids would not quench to a glass without water.

Compostions near 35 $CaCO_3$, 20 CaF_2, 25 $Ca(OH)_2$, 20 $BaSO_4$ produce a glass on quenching at 15,000 psi. pressure. The glasses appear to be stable at room temperature at atmospheric pressure. The liquidus temperature for this composition is near 650°C but devitrification can best be prevented by quenching from temperatures above this.

Contractor: Pennsylvania, University of, Philadelphia, Pennsylvania

Contract Number: AT(30-1)-1879

Present Contract Term: January 1, 1963 through December 31, 1963

Cost to AEC: $24,260

Contract Title: EFFECT OF PLASTIC STRESS ON DIFFUSION

Investigators: Robert Maddin

Scope of Work:

Since the research has two parts, I shall present two summaries.

Part 1

High purity gold foil (99.999) 0.01cm thick with a grain size of 0.01cm has been quenched from two temperatures, i.e. 980°C and 900°C at rates exceeding 10^5°C per sec. One of the foils (T_0 = 900) was annealed at 100°C for times up to one hour while the other was annealed at 174°C also for times up to one hour. Whereas the freshly quenched foils show no loops or tetrahedra, the specimens quenched and annealed show a larger number of tetrahedra. Curves of density of tetrahedra versus annealing time show an increase in density as a function of time. The density reaches a saturation value which appears to be characteristic of the quenching temperature and annealing temperature and time. The size of the tetrahedra, however, does not change with time. The higher quenching temperature results in a smaller tetrahedron size but a larger density.

Calculations show that the stacking fault tetrahedron grows (at 100°C) in times less than about three seconds. The calculations also indicate that the nucleation of the faults appears to be the rate controlling step in their formation. Activation energies of 1.22 ± 0.13 eV (T_0 = 980°C) and 1.05 ± 0.13 eV (T_0 = 900°C) have then calculated from these data.

During the remainder of this year and for half the next year, a series of quenching and annealing temperatures and times will be investigated. Calculations of the activation energy and critical size for the nucleus will be made.

Part 2

Silver single crystals sufficient to complete the research have been grown. Some of these crystals have been deformed in the twist-rest time experiments. The strain-anneal equipment has again been calibrated to insure dependable results. The diffusivities determined during the present research period after twisting and resting at high temperatures are slightly lower than those determined by C. H. Lee.

Being dissatisfied with previous sectioning techniques and taking cognizance of the possible error introduced in non-cylindrical cross-sections, G. Fisher has devoted considerable time to more accurate methods of sectioning. He has developed an electrolytic method capable of thin sections (on the order of one micron.) This method shows promise of allowing very accurate penetration curves and, at the same time, should answer the question of possible errors due to contour changes. The method will shortly be compared to one developed by Dr. C. T. Tomizuka and the more accurate method will be adopted.

Recent Publications:

C. H. Lee and R. Maddin, "Effect of Torsional Strains on Self-Diffusion in Silver," Journal Appl. Phys., Oct. 1961.

D. Kuhlmann-Wilsdorf, R. Maddin and W. Westdorp, "Unexpected Cross-Slip in Gold Foils," Journal Appl. Phys., Sept. 1962.

W. Westdorp and R. Maddin, "Nucleation of Stacking Fault Tetrahedra in Gold," Proc. Jap. Journal Phys. Int. Cong. Pure and Appl. Phys., Kyoto, Sept. 1962.

Contractor: Pennsylvania, University of, Philadelphia, Pennsylvania

Contract Number: AT(30-1)-1893

Present Contract Term: February 1, 1963 through January 31, 1964

Cost to AEC: $16,916

Contract Title: THE EFFECT OF STRESS ON RECOVERY

Investigators: Norman Brown

Scope of Work:

78% Ni-Fe Alloy (Permalloy)

A literature survey indicated that the mechanism wherely annealing twins form in f.c.c. metals was not known since the observations had been confined to optical microscopy. It was found that the annealing twins grew out of grain boundaries during the process of primary recrystallization. Thin packets of partial dislocations emanate from the grain boundary and increase the thickness of the twin in a direction perpendicular to the (111) twinning plane. Thus, the twin grows by the following processes: (1) the grain boundary adjacent to the twin migrates toward the unrecrystallized grain (2) partial dislocations nucleate at the grain boundary and glide on the (111) twinning plane (3) the partials extend by glide into the recrystallized grain and join together to form the non-coherent interface. In reality, the so called non-coherent interfaces often turn out to be coherent surfaces in that they are often the same plane in the twin as in the matrix. In this program, the growth of annealing twins is being studied using hot-stage, transmission electron microscopy. The relationship between the formation of annealing twins and martensite is being explored. The martensite reaction in various alloys of the type Fe-Ni, Fe-Ni-Co, and Fe, Ni, Cr are being investigated in order to determine the earliest stages in the formation of martensite.

beta Cu-Zn

Evidence for quenched-in vacancies has been observed in the βCu-Zn which has the CsCl structure. The evidence is based on the observation that during annealing of the quenched structure the dislocation density increases while the yield point and electrical resistivity decrease. Also the dislocations grow by the agglomeration of very small loops dislocations. This observation represents the first evidence concerning the existence of excess vacancies in a b.c.c. type crystal structure.

The work on βCu-Zn is a study of the transformation of vacancies to dislocations. There is an additional feature of interest because the dislocations are in the form of superlattice dislocations. Thus, the interaction of superlattice dislocations and vacancies will be investigated.

Recent Publications:

Norman Brown, "A Study of a Dilute Concentration of Disorder in the Beta Cu-Zn Superlattice," Accepted by Journal of Phys. & Chem. of Solids.

J. M. Roberts and N. Brown, "Low Frequency Internal Friction in Zinc Single Crystals," Acta Met., April, 1962.

J. M. Roberts and N. Brown, "Non-elastic Strain Recovery in Zinc Single Crystals," Acta Met. January, 1963.

Contractor: Pennsylvania, University of, Philadelphia, Pennsylvania

Contract Number: AT(30-1)-2395

Present Contract Term: February 1, 1963 through January 31, 1964

Cost to AEC: $96,858

Contract Title: OPTICAL AND MICROWAVE INVESTIGATIONS OF SOLIDS

Investigators: Elias Burstein

Scope of Work:

The research falls in three major areas: 1) Experimental investigation of the Fermi surface of metals, semimetals and semiconductors by means of Azbel'-Kaner type cyclotron resonance, magneto-acoustical resonance, deHaas-van Alphen oscillations, and transport properties. The materials under investigation include noble metals such as Au, transition metals such as Ni, bismuth, PbTe and Bi_2Te_3; 2) Electron tunneling phenomena in superconductors, such as Al, Sn and Pb, aimed at obtaining information about the lifetime of excited carriers, and in semiconductors such as InAs, PbTe and Bi_2Te_3, aimed at obtaining information about their energy band structures; 3) Infrared and Raman lattice vibration spectra of polar crystals such as LiH and LiD aimed at obtaining information about effective ionic charges, local fields and the role of anharmonicity and second order moments in these phenomena. In addition, there are related studies of the Stark effect on excitons in silicon and germanium; free carrier optical and acoustical activity and magneto-optical properties of Te and HgS; and photon- and Phonon-assisted tunneling in semiconductors and superconductors.

Recent Publications:

E. Burstein, D. N. Langenberg and B. N. Taylor, "Quantum Detection of Microwave and Sub-Millimeter-Wave Radiation Based on Electron Tunneling in Superconductors," Proceedings of the 1961 Quantum Electronics Conference.

P. J. Stiles, E. Burstein and D. N. Langenberg, "Observations of de Haas-van Alphen Oscillations in p-type PbTe," Phys. Rev. Letters 6, (1961) p. 511.

P. J. Stiles, E. Burstein and D. N. Langenberg, "de Haas-van Alphen Effect in p-type PbTe and n-type PbS," J. of Appl. Phys. Supp. 32, (1961) p. 2174.

A. S. Filler, "Primary Aberrations of Mirrors," Amer. J. of Phys. 29, (1961) p. 687.

A. S. Filler and L. Indyk, "Calibration of Infrared Prism Spectrometers," J. of Optical Soc. of Amer. 51, (1961) p. 572.

Contractor: Pittsburgh, University of, Pittsburgh, Pennsylvania

Contract Number: AT(30-1)-647

Present Contract Term: September 1, 1962 through August 31, 1963

Cost to AEC: $32,689

Contract Title: APPLICATION OF CHEMICAL THERMODYNAMICS AND RELATED PHENOMENA TO THE STUDY OF ALLOY FORMATION

Investigators: W. E. Wallace

Scope of Work:

The general objective of the present work is to further our understanding of solids in general and metals in particular by studying the constitution, thermal properties and magnetic and electrical behavior of selected systems. Emphasis is currently being placed on lanthanide hydrides and nitrides. Intermetallic compounds between the lanthanide metals and manganese are also being studied to some extent. Specific systems which are being or will be studied are: 1) Pr, Nd and Sm hydrides, 2) HoD_2, TbD_2 and HoD_3, 3) NdH_2, 4) EuH_2, 5) the lanthanide nitrides and 6) compounds and alloys represented by the formulas LMn_2 and $LMn_{2-x}Al_x$, in which L represents a lanthanide metal.

The character and objectives of the work are as follows: 1 and 5 - magnetic studies to ascertain whether these substances order magnetically at low temperatues; 2 - neutron diffraction work to ascertain chemical and magnetic sturctures; 3 - neutron diffraction and low temperature heat capacity work to reveal possible crystal field effects; 4 - electrical conductivity to determine whether EuH_2 is metallic or ionic; 6 - structures and magnetic properties surveyed in the light of alloy theory. 1, 3 and 4 are providing detailed information regarding the bonding in the lanthanide hydrides.

Recent Publications:

W. G. Saba, W. E. Wallace, H. Sandmo, and R. S. Craig, "Heat Capacities and the Residual Entropy of Ta_2H," J. Chem. Phys., 35, (1962) p 2148.

William G. Saba and W. E. Wallace, "Heat Capacities of $DyCo_5$ in the Region of its Magnetic Anomaly and Third Law Entropies," J. Chem. Phys., 35, (1961) p. 689.

W. E. Wallace, P. Kofstad, and L. J. Hyvönen, "Transformation in the Ta-H and Ta-D Systems," Pure and Appl. Chem., 2, (1961) p. 281.

M. V. Milnes and W. E. Wallace, "The Residual Entropy of the Equimolal KCl-KBr Solid Solution in Relation to Wasastjerna's Theory of Alkali Halide Solid Solutions," J. Phys. Chem., 65, (1961) p. 1456.

W. E. Wallace, "Neutron Diffraction Data for Ta_2D and the Probable Arrangement of the Deuteriums in Two of Its Polymorphic Varieties," J. Chem. Phys., 35, (1962) p. 2156.

A. Pebler and W. E. Wallace, "Crystal Structures of Some Lanthanide Hydrides," J. Phys. Chem., 66, (1962) p. 148.

R. L. Zanowick and W. E. Wallace, "Ferromagnetism in EuH_2," Accepted by Phys. Rev.

Y. Kubota and W. E. Wallace, "Magnetic Characteristics of Hydrogenerated Holmium," J. Appl. Phys., 33, (1962) p. 1348.

R. L. Zanowick and W. E. Wallace, "Constitution and Magnetic Susceptibilities of Vanadium-Hydrogen Alloys," Accepted by J. Chem Phys.

W. E. Wallace, Y. Kubota and R. L. Zanowick, "The Magnetic Characteristics of Gadolinium, Terbium and Ytterbium Hydrides in Relation to the Electronic Nature of the Lanthanide Hydrides," Accepted by J. Inorg. Chem.

Contractor: Pittsburgh, University of, Pittsburgh, Pennsylvania

Contract Number: AT(30-1)-2163

Present Contract Term: May 1, 1963 through April 30, 1964

Cost to AEC: $43,923

Contract Title: CALORIMETRIC, STRUCTURAL AND MAGNETIC STUDIES OF METALS AND INTERMETALLIC COMPOUNDS

Investigators: Raymond S. Craig

Scope of Work:

The following problems are under investigation:

1. A study of the magnetic and structural characteristics of solid solutions of dysprosium in yttrium, holmium in yttrium, and terbium in yttrium.

2. Heat capacity measurements in the temperature range 1.5 to 4°K on the following systems:

(a) $TiFe_2$ - $ZrFe_2$
(b) $ZrFe_2$ - $ZrCo_2$
(c) Dilute solid solutions of Mg and Cd

3. An investigation of the effect of occluded oxygen and/or nitrogen on the magnetic properties of $TiFe_2$.

4. We intend to carry out some extensive improvements to our calorimetric facilities for the temperature range 10 to 300°K. Upon the completion of the equipment modifications we plan to measure the specific heats of europium and α-manganese.

Recent Publications:

R. A. Butera, R. S. Craig, and L. V. Cherry, "Electromagnetic Servo-Balance Employing a Differential Transformer," Rev. Sci. Inst. 32, (1961) p. 708.

W. G. Saba, W. E. Wallace, H. Sandmo, and R. S. Craig, "Heat Capacities and the Residual Entropy of Ta_2H," J. Chem. Phys. 35, (1961) p. 2148.

W. G. Saba and W. E. Wallace, "Heat Capacities of $DyCo_5$ in Relationship to Its Magnetic Anomaly, Third Law Entropies, and Related Thermochemical Data," J. Chem. Phys. 35, (1961) p. 689.

Contractor: Princeton Universtiy, Princeton, New Jersey

Contract Number: AT(30-1)-2680

Present Contract Term: November 1, 1962 through October 31, 1963

Cost to AEC: $87,865

Contract Title: LATTICE AND ELECTRONIC DEFECTS IN SOLIDS

Investigators: R. Smoluchowski

Scope of Work:

Alkali Halides

Studies have been made on the effect of plastic deformation on the low temperature ionic conductivity. The data obtained was inconclusive as far as determining the effect of oriented dislocations on the activation energy of ionic motion was concerned but it seems that the data obtained can best be understood in terms impurity precipitation and relocation during the deformation process. In conjunction with these deformation experiments etch pit measurements have been made to determine the number of dislocations introduced by deformation. On the average this number agrees with theoretical prediction.

The mechanism of introducing point defects by ionizing radiation has also been studied experimentally. Initial measurements using white x-rays, having maximum energies just above and below the K ionization threshold for chlorine have indicated that a Varley type process is probably important in the formation of defects at liquid nitrogen temperatures although the data would indicate that other mechanisms are also operative.

Silver Halides

A theory for transient polarization currents in insulators has been developed and tested experimentally using AgCl. The technique has been demonstrated to be a powerful tool for investigating traps in crystals and the interaction of these traps with phonons.

Theory

Electron-phonon interactions in metals have been studied and an expression for the attenuation of sound waves developed. This agrees with the experimental results of Pippard.

Electron-Donor recombination in semiconductors has also been investigated and it has been shown that recombination via capture in an excited state is important at helium temperatures and low electron densities whereas impact recombination dominates at higher electron concentrations.

The anomalous electrical resistivity of α and stabilized δ plutonium has been explained in terms of interband scattering and a band structure proposed that can account for the observed phenomena including the effects of alloying. The fractional valence of certain cerium allotropes has been explained in terms of an antiferromagnetic structure for both the α and δ phases.

Recent Publications:

R. Smoluchowski, M. Merriam and D. A. Wiegand, "Enhanced Thermal Expansion in KCl," Phys. Rev. 125, (1962) p. 52.

R. Smoluchowski, M. Merriam and D. A. Wiegand, "High Temperature Thermal Expansion in NaCl," Phys. Rev. 125, (1962) p. 65.

R. Smoluchowski, "Problem of Anomalous Resistivity of Plutonium," Phys Rev. 125, (1962) p. 1577.

R. Smoluchowski and J. Sharma, "Enhanced Colorability of KCl at K-ionization Limit," Bull. Am. Phys. Soc. (II) 7, (1962) p. 178.

R. Smoluchowski and B. S. H. Royce, "Oriented Dislocations and Ionic Conduction of KCl," Bull. Am. Phys. Soc. (II) 7, (1962) p. 210.

R. Smoluchowski and K. Gschneidner, "Valences of Cerium Allotropes" Bull. Am. Phys. Soc. (II) 7, (1962) p. 230.

P. J. Warter, Jr. and G. Warfield, "Short Term Transient Currents in Insulators with Blocking Electrodes," Am. Physical Soc. Bull. 7, (1962) p. 178.

P. J. Warter, Jr. and G. Warfield, "Transient Polarization in the Presence of Non-Injecting Contacts" Report on Conference on Space Charge effects in Dielectrics, Westhampton Beach, Long Island, June, 1962.

G. Heilmeier, G. Warfield and S. E. Harrison, "Measurements of Hall Effects in Metal-Free Phthalocyanine Single Crystals" Phys. Rev. Let. 8, (1962) p. 308.

S. Rodriguez and G. Ascarelli, "Recombination of Electrons and Donors in Semiconductors" J. Phys. Chem. Solids 22, (1961) p. 57.

S. Rodriguez and G. Ascarelli, "Recombination of Electrons and Donors in n-type Germanium" Phys. Rev. 124, (1961) p. 1321.

S. Rodriguez and G. Ascarelli, "Recombination of Electrons and Donors in n-type Germanium, Part B" Phys. Rev. (July 1962).

G. Warfield and P. J. Warter, Jr., "Polarization Currents Associated with the Thermal Release of Trapped Electrons in AgCl Crystals," Am. Phys. Soc. Bull 7, (1962) p. 179.

S. Rodriguez, "Impact Capture of Electrons my Donors," Bull. Am. Phys. Soc. 7, (1962) p. 232.

S. Rodriguez and K. Tharmalingam, "Attenuation of Phonons by an Electron Plasma" Bull. Am. Phys. Soc. 7, (1962) p. 192.

Contractor:	Puerto Rico Nuclear Center, Rio Piedras, Puerto Rico
Contract Number:	AT(40-1)-1833
Present Contract Term:	February 1, 1963 through June 30, 1963 (Part of FY-1963)
Cost to AEC:	$11,000
Contract Title:	STUDY OF RADIATION DAMAGE IN ORGANIC CRYSTALS USING ELECTRICAL CONDUCTIVITY
Investigators:	Amador Cobas and H. Harry Szmant

Scope of Work:

This is a new project concerned with the effects of radiation on organic crystals. In particular, the effect of neutron and of gamma and X-ray irradiation on the electrical conductivity of anthracene crystals will be studied. Because electrical conductivity is most sensitive to the presence of impurities or defects, it should become possible to detect quantitatively radiation damage at levels far lower than those that can be observed by other chemical or physical techniques. Correlation of the electrical properties directly with optical and other properties of the crystal will be attempted.

The initial stage of this investigation is being limited to the study of the changes in dark and photoconductivity in anthracene crystals produced by neutron bombardment. This type of irradiation may produce a single type of defect, namely, the knocking out of a hydrogen atom from the anthracene molecule. It is likely that a result of the condensed aromatic system and it is planned to investigate this possibility by spectroscopic examination of the crystal between successive neutron bombardments, and finally by a high temperature adaptation of vapor phase chromatography of the repeatedly exposed crystals. The spectroscopic examination of the crystals may also detect any oxidative changes at the crystal surface.

Information on trap densities can be related, as indicated previously, to the concentration of defects and the knowledge of trap depths can be related ultimately to the chemical nature of the molecular species produced by irradiation.

A future phase of this investigation will include the more precise and direct technique of determining trap densities and depths by measuring mobility and conductivity as a function of temperature.

Similar studies will be made with other organic crystals.

Contractor:	Puerto Rico Nuclear Center, Mayaguez, Puerto Rico
Contract Number:	AT(40-1)-1833
Present Contract Term:	February 1, 1963 through June 30, 1963 (Part of FY-1963)
Cost to AEC:	$85,000
Contract Title:	NEUTRON DIFFRACTION STUDIES OF THE STRUCTURAL ROLE OF HYDROGEN IN CRYSTALS AND OF MAGNETIC SPIN ARRANGEMENTS IN INORGANIC CRYSTALS
Investigators:	I. Almodóvar

Scope of Work:

The neutron diffraction program at Puerto Rico Nuclear Center is concerned in general with ideal and imperfect arrangements of atomic nuclei and magnetic spin systems in solids. In particular, interest is centered on the determination of the role of hydrogen and oxygen in structures of importance to solid state physics and chemistry and on the determination of the magnetic structures of inorganic salts.

Problems first considered in this new program have been structural determinations of $CaWO_4$ (scheelite), $BaNiO_2$ and Fe_2SiO_4. Work has been completed on the first and is being continued on the next two and other isomorphous crystals.

New projects to be started soon involve determination of the role of hydrogen in the solid phases of compounds such as methanol and dimethyl acetylene which are not solid at room temperature, and in copper formate tetrahydrate ($Cu(HCO_2)_2 4H_2O$) and $KPtCl_3NH_3$. Also the magnetic spin arrangements in thiospinels will be sought.

Contractor: Purdue University, Lafayette, Indiana

Contract Number: AT(11-1)-125

Present Contract Term: April 1, 1963 through March 31, 1964

Cost to AEC: $76,969

Contract Title: BASIC RADIATION DAMAGE STUDIES

Investigators: H. M. James and H. Y. Fan

Scope of Work:

The proposed work is a continuation of investigations directed toward attaining an understanding of the basic processes of radiation damage in semiconductors, particularyly germanium. Thus far, the major tool has been measurements of electrical properties of irradiated crystals; these are, however, supplemented by calorimetric measurements of the stored energy released as defects anneal, and electron spin resonance studies will soon begin. Irradiation at liquid helium temperatures by electrons in the energy range 0.5 to 1.0 Mev has proved to be most informative for investigations of defect formation. Irradiation and annealing studies have revealed that the only defect produced directly by a collision of an electron with a lattice atom under these conditions is an unstable defect that anneals at 65^{o}K. This defect can be transformed to a stable defect, or it may be caused to anneal, by either radiation or thermally induced excitation of the crystal. Since all stable defects produced under the conditions studied here are formed from this unstable defect, an understanding of its structure and dynamics is fundamental to an understanding of radiation damage processes in germanium. We plan to study its structure by electron spin resonance, and we are studying the dynamics, seen as a rate effect at liquid nitrogen temperature; stored energy released as the specimen is annealed; temperature dependence of defect production. This work will be extended to similar studies of silicon if new personnel becomes available.

Recent Publications:

J. A. Haber and H. M. James, "Effect of Hydrogen on the Displacement Processes in Ge," Bull. Am. Phys. Soc. 6, (1961) p. 303.

E. E. Klontz and J. W. MacKay, "Low Temperature Annealing of Electron-Bombarded Ge," Bull. Am. Phys. Soc. 6, (1961) p. 303.

Contractor: Purdue University, Lafayette, Indiana

Contract Number: AT(11-1)-359

Present Contract Term: April 1, 1962 through March 31, 1963

Cost to AEC: $6,842

Contract Title: DIFFUSION IN LIQUIDS AND SOLIDS

Investigators: Richard E. Grace

Scope of Work:

The current research programs can be classified into two main categories. The first deals with volume diffusion in ternary metallic solid solutions and in metal oxides, and the second category deals with heterogeneous gas-solid reactions. The following problems are being studied:

1. Diffusion paths and interdiffusion coefficients are being investigated in copper-rich solid solutions of copper-zinc-manganese alloys. A variational method of analyzing diffusion paths has been proposed, and experimental work on diffusion of zinc and manganese from the vapor phase into copper has begun.

2. Self-diffusion of chromium in single crystal disks of Cr_2O_3 is being studied. The disks are equilibrated before and during the diffusion anneal with controlled atmospheres of damp hydrogen in order to control the concentration of crystal defects. The results are to be correlated with oxidation studies of metallic chromium which have recently been completed.

3. Reduction of metal oxides under conditions not far removed from equilibrium will be studied with a gravimetric microbalance technique. Reduction of wustite in damp hydrogen will be investigated under conditions where the Gibbs free energy change will be the order of 1 Kcal/mole or less.

Recent Publications:

Richard E. Grace, "Rates of Solution of Rotating Zinc Cylinders in Liquid Bismuth," AIME, Phys. Chem. of Process Metallurgy Part I, Interscience Publishers, New York (1961) pp. 633-644.

Contractor: Minnesota, University of, Minneapolis, Minnesota

Contract Number: AT(11-1)-532

Present Contract Term: June 1, 1962 through May 31, 1963

Cost to AEC: $26,108

Contract Title: EFFECT OF ATOMIC RADIATION AND OF MOLECULAR ORIENTATION ON MECHANICAL BEHAVIOR OF LINEAR SOLID HIGH POLYMERS

Investigators: C. C. Hsiao

Scope of Work:

During this coming year, it is planned to study the role of macromolecular orientation and the strength of polymeric solids. Correlations between deformation and anisotropic strength will be made. Related topics such as branching and perhaps cross-linking will be considered. An attempt will be made to develop a generalized viscoelastic stress-strain law incorporating the nature of macromolecular orientation in the creep and relaxation functions. If possible, some simple axisymmetrical anistropic, non-homogeneous viscoelastic stress analysis problems will be investigated under steady state temperature field.

In addition, using explosives the short time dependent fracture strength of some polymeric solids will be studied in the microsecond regions. It is hoped that this will be carried out for oriented samples at different temperatures.

Recent Publications:

C. C. Hsiao and J. W. Yang, "Effect of γ-Irradiation on Strength of Oriented Polyethylene" Technical Rpt. # 13, AEC # 532, (1961) pp. 1-19.

C. C. Hsiao and T. S. Wu, "Analysis of Orientation and Strength of Branched Polymer Model Solid," Technical Rpt. # 14, AEC # 532, (1961) pp. 1-20.

C. C. Hsiao, "A Theory for the Effect of Plastic Deformation on Elastic Behavior of a Model Solid," Technical Rpt. # 15, AEC # 532, (1961) pp. 1-57.

C. C. Hsiao and J. C. Das, "Some Elementary Aspects of Wave Propagation in Viscoelastic Bar," Technical Rpt. # 16, AEC # 532, (1961) pp. 1-23.

Recent Publications:

C. C. Hsiao, J. E. Osborn and D. B. Rozendal, "Orientation Dependent Mechanical Breakdown of a Model High Polymer Solid," J. Phy. Soc. of Japan, Vol. 16, No. 3, (1961) pp. 459-462.

C. C. Hsiao, J. E. Osborn, "Uniaxial Deformation Dependent Mechanical Strength of a Model Solid," Proceedings of the 10th Japan National Congress for Applide Mechanics, (1961) pp. 11-13.

Contractor: Minnesota, University of, Minneapolis, Minnesota

Contract Number: AT(11-1)-841

Present Contract Term: November 1, 1962 through October 31, 1963

Cost to AEC: $36,392

Contract Title: DIFFUSION STUDIES IN LIQUID METALS

Investigators: Richard A. Swalin

Scope of Work:

In order to help validate a proposed mechanism of diffusion, the atomic mobility of the series cadmium, indium, tin and antimony in liquid silver is to be obtained. To date, the diffusivity of silver in silver and of tin in silver have been measured and results are in general quantitative agreement with a fluctuation theory of diffusion based on the known energetics of solute-solvent ions in the above systems. In addition to this activity research work is being initiated on various properties of sodium and potassium. In particular, self-diffusion, Hall effect and electrical resistivity are to be investigated as a function of temperature and pressure in order to obtain these properties at constant volume. From these studies useful information about the nature of volume fluctuations in the liquid may be obtained.

For example our model leads to the prediction that tin should diffuse 31% faster than silver ions in silver. From experimental studies we find that tin diffuses 34% faster.

Recent Publications:

R. A. Swalin, "Fluctuation Theory of Liquids," Submitted to Acta Met.

R. A. Swalin and C. H. Ma, "Self-Diffusion in Liquid Tin," To be published Jnl. of Chem. Physics.

Contractor:	Minnesota, University of, Minneapolis, Minnesota
Contract Number:	AT(11-1)-1009
Present Contract Term:	March 16, 1962 through March 15, 1963
Cost to AEC:	$17,611
Contract Title:	A STUDY OF THE ANOMALOUS RESISTIVITY CHANGE ACCOMPANYING PLASTIC DEFORMATION IN Cu-Pd and Ag-Pd ALLOYS
Investigators:	Morris E. Nicholson

Scope of Work:

Work to date has shown short-range order exists in the Au-Pd system. This order is destroyed when these alloys are cold worked. The amount of short-range order will be determined in a series of Au-Pd alloys using X-ray diffuse scattering techniques. In addition, a study will be made of this rate at which order is destroyed by cold work and the rate at which order is re-established by low temperature annealing. This work will be correlated with the change in resistivity, Hall constant and mobility resulting from cold working or annealing.

A study of the change in resistivity as a function of pressure will be made for a series of Ag-Pd alloys after being cold worked to various degrees. A study will be initiated of the change in resistivity, Hall constant and mobility upon cold working with composition where Cu is substituted for Ag in Ag-Pd alloys.

Contractor:	Mississippi, University of, University, Mississippi
Contract Number:	AT(40-1)-2891
Present Contract Term:	June 15, 1962 through September 14, 1963
Cost to AEC:	$47,149
Contract Title:	THE EFFECTS OF NEUTRON IRRADIATION ON THE ELECTRONIC PROPERTIES OF BINARY ALLOYS
Investigators:	A. B. Lewis

Scope of Work:

Construction of a shielded building has been completed and a Dynamitron particle accelerator, capable of producing monenergetic neutrons by positive ion bombardment of tritium, has been installed. Alloys will be irradiated at differing temperatures and changes in internal structure will be determined in the following ways: a) Resistivity measurements will be made on samples of varying atomic percentages across a solvus phase boundary. b) For samples having percentage compositions lying near the phase boundary at a given temperature, resistivity measurements will be made at various temperatures extending vertically on the phase diagram across the phase boundary. c) Attempts will be made to determine if frozen-in defects in samples of Cu-Al (15% Al) annealed from around 300°C to room temperature will cause a change in resistivity on being irradiated.

Contractor:	National Bureau of Standards, Washington, D.C.
Contract Number:	NBS Project No. 0905-11-09450
Present Contract Term:	July 1, 1962 through June 30, 1963 (Fiscal Year 1963)
Cost to AEC:	$60,000
Contract Title:	INFLUENCE OF THE ATMOSPHERE ON PERFECTION OF CRYSTALS GROWN BY THE VERNEUIL TECHNIQUE
Investigators:	W. S. Brower

Scope of Work:

The objective of this program is to determine the influence of the atmosphere and thermal environment on the perfection of crystals, such as TiO_2, ferrites, titanates and other high melting substances, grown by the Verneuil technique. Methods of growing such crystals with control over the impurity and defect population are being developed.

The plasma-torch modification of the Verneuil process is being exploited for preparing crystals, such as TiO_2, in which control of the hydrogen content has current scientific importance. So far, growth of TiO_2 crystals in the plasma torch, fed by ordinary argon and oxygen, has shown no reduction in hydrogen content. In a program to grow refractory crystals by the plasma torch method, crystals of stabalized ZrO_2, Y_2O_3, and Cr_2O_3 have been grown.

The utilization of direct electromagnetic heating to grow refractory crystals is being planned. A special, high power multifrequency VHF generator has been ordered and built for this purpose.

Etching techniques are being developed and used for the evaluation of the crystals grown by the various techniques. Successful techniques for Cr_2O_3 have been found.

The precipitation of Al_2O_3 in TiO_2 crystals is being studied in order to evaluate the diffusion of Al_2O_3 in TiO_2.

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Ames(Met) A-1, -3
Ames(SS) 1, 2
ANL(Met) A-2; B-2, -3, -4, -5, -8
A I, A
BMI(Rudman)
BNL(Met) B-2
Cal U(Berk)(Dransfeld) AT(11-1)-34 #76
Calif(LRL) A-4, C
Case(Hehemann) AT(30-1)-3033
Del U(Skolnik) AT(30-1)-2722
Ill U(Maurer) II A AT(11-1)-1198
Ill U(Sinclair) AT(11-1)-1046
MIT(Pearsall)
MIT(Shull) AT(30-1)-3031
NBS(Frederikse) #13443
Okla U(Daniels) AT(40-1)-2570
Penn St(Gingerich) AT(30-1)-2541
Temple(Salomon) AT(30-1)-2780
Toledo(Zmeskal) AT(11-1)-1000
U C(Met) B-1, -2, -3; D-1; E-1
Union Carbide(Met) C-5
VPI(Eckel) AT(40-1)-2564

Group VI transition metals - Cr, Mo, W, pure, alloyed, and in compounds
Ames(Met) A-1, -3
Ames(SS) 1
ANL(Met) A-2, -4
BNL(Met) A-1
Calif(LRL) C
Col U(Machlin) AT(30-1)-2921
HAPO(Rad Damage)
Ill U(Maurer) II A AT(11-1)-1198
NBS(Brower) 0905-11-09450
N West U(Wagner) AT(11-1)-1126
Penn St(Bell) AT(30-1)-2581
Penn St(Gingerich) AT(30-1)-2541
Penn St(Tuttle) AT(30-1)-2887
Purdue(Grace) AT(11-1)-359
RIAS(Otte) AT(30-1)-2531
Tenn U(Stansbury) AT(40-1)-1068
U C(Met) B-1, -3

H

Halides
Ala U(Carlson) AT(40-1)-3090
Ames(Met) A-1; B-3
Ames(SS) 3, 6
ANL(SS) A-1, A-2b, A-2c, A-3; B-3a; C-2; E-d
Ariz St(Gossick) AT(11-1)-715
Ark U(Sharrah/Kruh) AT(40-1)-2096
ARF(Markham) AT(11-1)-578 Proj No 9
BNL(SS) B-2
Brn U(Bray) AT(30-1)-2024
Cal U(Berk)(Portis) AT(11-1)-34 Proj #47
Cal U(Berk)(Dransfeld) AT(11-1)-34 #76
Calif(LRL) A-3; B-3
Cal(Riv)(Satten)
Carn(Bauer) AT(30-1)-3001
Carn(Wiegand) AT(30-1)-3033
Case(Smith) AT(11-1)-623
Chi U(Rice) AT(11-1)-357
C U(Sproull/Krumhansl) AT(30-1)-2391
C U(Sack) AT(30-1)-2471
C U(Che-Yu Li) AT(30-1)-3228
IIT(Grossweiner) AT(11-1)-1052
Ill U(Maurer) II C, III A, F AT(11-1)-1198
IBM(Nowick) AT(30-1)-2811
Kans U(Friauf) AT(11-1)-1197
Md U(Schamp) AT(40-1)-2068
MIT(King) AT(30-1)-1985
MSU(Wei) AT(11-1)-1042
NBS(Frederikse) #13443
Neb U(Pearlstein) AT(11-1)-525
NCU(Slifkin) AT(40-1)-2036
Princt U(Smoluchowski) AT(30-1)-2680
RPI(Casabella) AT(30-1)-3030
Union Carbide(Met) A-1; C-1; D-2
Union Carbide(SS) D-1, -2, -3, -5
Utah(Ohlsen) AT(11-1)-1284
Va U(Catlin) AT(40-1)-3012
Wake F(Turner/Williams) AT(40-1)-2413
Wayne St(Kim) AT(11-1)-1054
Yale(Robertson) AT(30-1)-2723

High Temperature Mechanical Properties, Creep
Cornell Univ(Ruoff) AT(30-1)-2504
Stanf(Sherby) AT(04-3)-326 #2

Hydrogen - in solid solution, hydrides, deuterides, tritides, reaction with solids
Ames(Met) B-2, -3
ANL(Met) A-5; C-2; E-2
ANL(SS) B-2
Chi U(Rice) AT(11-1)-357
Gen Mls(Wehner) AT(11-1)-722
Oklahoma U(Daniels) AT(40-1)-2570
PRNC(Almodovar) AT(40-1)-1833
Purdue(Grace) AT(11-1)-359
Tenn U(Stansbury) AT(40-1)-1068
Tufts(Handler) AT(30-1)-2968
Vt U(Flanagan) AT(30-1)-3000
West(Gulbransen)

I

Impurities and dopants, distribution and effects
Ala U(Carlson) AT(40-1)-3090
Ames(Met) A-3
ANL(Met) A-2; D-2
ANL(SS) A-1, -2, -3; B-1
Ariz U(Tomizuka) AT(11-1)-1041
BNL(Met) A-1
BNL(SS) A-4, b, c; B-2
Carn(Bauer) AT(30-1)-3001

L

M

N

O

JHU(Bearden) AT(30-1)-2185 and 2543
Little, Arthur D Inc(Davis) AT(30-1)-2756
MIT(King) AT(30-1)-1985
MIT(Kingery) AT(30-1)-2574
NBS(Brower) 0905-11-09450
NDU(Bale) AT(11-1)-1255
Northwestern Univ(Wagner) AT(11-1)-1126
ORNL(Met) A-1; C-1; D-1, -3; E-1
Penn State(Bell) AT(30-1)-2581
Penn State(Muan)
Penn State(Tuttle) AT(30-1)-2887
PRNC(Almodovar) AT(40-1)-1833
Purdue(Grace) AT(11-1)-359
RPI(DeVries/Ansell) AT(30-1)-3176
Stanford Univ(Sherby)
Temple(Salomon) AT(30-1)-2780
Union Carbide Nuclear Co(SS) C-6; D-3, -4
Utah Univ of(Cutler) AT(11-1)-1122
Utah(Ohlsen) AT(11-1)-1284
Wayne St(Kim) AT(11-1)-1054

P

Paramagnetism - See Magnetic properties

Phase Relations in metallic and non-metallic systems at equilibrium
Ames(Met) B-2
ANL(Met) B-1, -6, -7; C-2a
Armour Res Foundation(Elliott) AT(11-1)-578 #19
BNL(Met) A-1
Calif U of(LRL) B-2; C-1
CIT(Duwez) AT(04-3)-221
Denver Univ of(Colorado Seminary) (Nachman/Lundin)
Ill Univ of(Sinclair)
MIT(Ogilvie) AT(30-1)-3134
Mellon(Massalski) AT(30-1)-2684
NYU(Komarek) AT(30-1)-2916
Penn State(Bell) AT(30-1)-2581
Penn St(Muan) AT(30-1)-2781
RPI(Burr) AT(30-1)-2159
Stanford Univ(Stevenson) AT(04-3)-283
Syracuse Univ(Kanda/King) AT(30-1)-1910
Syracuse Univ(Kanda/Keller) AT(30-1)-2731
Union Carbide Nuclear Co(Met) B-1, -3
Vermont Univ of(Flanagan) AT(30-1)-3000
VPI(Eckel) AT(40-1)-2564
Westinghouse Electric Corp(Gulbransen)
Yale Univ(Robertson) AT(30-1)-2723

Phase transformations, mechanisms, and kinetics (Melting & solidification listed separately)
And U(Snyder) AT(11-1)-976
ANL(Metallurgy) A-1, -4
ANL(SS) B-3a
Calif U of(Berkeley) A-3; B-1, -2
Cal(Riv)(Lawson) AT(11-1)-34 #77
Case(Heheman) AT(11-1)-588
Hanford Atomic Products Operations(Pu) AT(45-1)-1350
Ill U(Maurer) IV A, B, C
Mellon(Massalski) AT(30-1)-2684
Penn St(Gingerich) AT(30-1)-2541
Penn U(Brown) AT(30-1)-1893
RPI(Burr) AT(30-1)-2159
RIAS(Otte) AT(30-1)-2531
Stanford Univ(Sherby) AT(04-3)-326 #2
VPI(Leinhardt) AT(40-1)-2689
Wash Univ of(Polonis) AT(45-1)-1375

Phonons - See lattice vibrations

Phosphides, arsenides, and sulfides
Cal(Riv)(Lawson) AT(11-1)-34 #77
Carn(Philbrook) AT(30-1)-2360
NBS(Frederikse) #13443
Penn St(Gingerich) AT(30-1)-2541
U C(Met) E-1
U C(SS) B

Photon irradiation (gamma rays, x-rays, light, ie. all electromagnetic irradiation)
ANL(SS) A-1; C-2
Ariz St(Gossick) AT(11-1)-715
B & L(Kreidl) AT(30-1)-1312
BNL(SS) A-1, -3; B-2
Carn(Bauer) AT(30-1)-3001
Conn U(Gilliam) AT(30-1)-2047
IIT(Grossweiner) AT(11-1)-1052
Ill U(Maurer) II C AT(11-1)-1198
Kansas U(Friauf) AT(11-1)-1197
MIT(Mason/Reid) AT(30-1)-2909
Neb U(Pearlstein) AT(11-1)-525
Princeton(Smoluchowski) AT(30-1)-2680
PRNC(Cobas/Szmant) AT(40-1)-1833
RPI(Casabella) AT(30-1)-3030
U C(SS) D-1
Wayne St(Kim) AT(11-1)-1054

Plastic Deformation - See Deformation and Dislocation Studies

Plutonium - See Actinides

Positron annihilation
Ames, SSdw 1
WRU(McGervey) AT(11-1)-1297

Positive ion bombardment effects
ANL(SS) C-2
Gen Mills(Wehner) AT(11-1)-722
Houston(Reynolds) AT(40-1)-2573
Mississippi(Lewis) AT(40-1)-2891
Neb U(Pearlstein) AT(11-1)-525
U C(SS) C-4

Precipitation
ANL(Met) D-5
A I - B
BNL(SS) A-2
Brown U(Bray/Hooper) AT(30-1)-2024
Case(Hehemann) AT(11-1)-588
Cinci U(Hoch/Meeks) AT(11-1)-1115
C U(Silcox) AT(30-1)-3087
Ill U(Maurer) IV C, D AT(11-1)-1198
NBS(Brower) 0905-11-09450
RPI(Ansell/DeVries) AT(30-1)-3176
Wash Univ of(Polonis) AT(45-1)-1375
Yale Univ of(Robertson) AT(30-1)-2723

Pressure Effects
Ames - SS dw 1, 3, 5, 6
ANL(SS) Ea
Arizona U of(Tomizuka) AT(11-1)-1041
B & L(Kreidl) AT(30-1)-1312
Calif U of(Lawson) AT(11-1)-34 #77
Case(Smith) AT(11-1)-623
Chicago U of(Rice) AT(11-1)-357
Cornell Univ(Ruoff) AT(30-1)-2504
Illinois U of-H-(Maurer) II A, E, F III B AT(11-1)-1198
MSU(Schamp) AT(40-1)-2068

Minn U(Swalin) AT(11-1)-841
Minn U(Nicholson) AT(11-1)-1009
Penn St(Tuttle) AT(30-1)-2887

Purification
Ames(Met) #1(Spedding) W-7405-Eng-82
ANL(Met) A-4, -5
Materials Res Corp(Abowitz)
Union Carbide Corp(Westbrook)

R

Radiation Damage and Radiation Effects
ANL(Met) C-5; D-1, -2, -3, -4, -5; F-1
ANL(SS) A-1; A-2c; B-1, -2; C-2
Arizona State(Gossick) AT(11-1)-715 A I - C
Bausch & Lomb Inc(Kreidl) AT(30-1)-1312
BNL(Met) B-1, -2, -3; C-2, -3
BNL(SS) A-1, -2, -3, -4a; B-2
Brown U(Bray/Hooper) AT(30-1)-2024
Carn(Bauer) AT(30-1)-3001
Carnegie I T(Wiegand) AT(30-1)-3033
Chi U(Rice) AT(11-1)-357
Clemson College(Chaplin) AT(40-1)-2098
Connecticut U(Gilliam) AT(30-1)-2047
Cornell Univ(Webb/Silcox) #3029
Cornell Univ(Silcox) #3087
Cornell Univ(Silsbee/Bowers) AT(30-1)-2150
Franklin Inst(Pomerantz) AT(30-1)-2730
General Mills(Wehner) AT(11-1)-722
HAPO(Rad Effects) AT(45-1)-1350
Hstn U(Reynolds/Allred) AT(40-1)-2573
Illinois Univ of -C-(Koehler) AT(11-1)-1198
Kansas Univ of(Friauff)
MIT(Mason/Reid) AT(30-1)-2909
MIT(Simnad/Uhlig)
Mass Univ of(Stein) AT(30-1)-3003
Mississippi Univ of(Lewis) AT(40-1)-2891
Nebraska Univ of(Pearlstein)
N Carolina Univ of(Shearin) AT(40-1)-2577
North Dakota(Bale) AT(11-1)-1255
Northwestern Univ(Kauffman) AT(11-1)-1161
Penn State(Sauer)
Penn State(Diethorn/Walker) AT(30-1)-2792
Puerto Rico Nuclear Centre(Cobas/Szmant) (AT(40-1)-1833)
Purdue(James) AT(11-1)-125
RPI(Brown) AT(30-1)-1995
RPI(Casabella) AT(30-1)-3030
RPI(Huntington) AT(30-1)-1995
Union Carbide(Met) D-3
Union Carbide Co(SS) A-1, -2, -3, -4; B; C-2, -3, -4, -5, -6; D-1, -2, -3, -4, -5
Utah Univ of(Ohlsen) AT(11-1)-1284
Wayne State(Kim)

Rare Earths and Rare Earth Compounds
Alabama Univ of(Carlson) AT(40-1)-3090
Ames(Met) B-2, -3
Ames, SS dw 1, 2, 4
ANL(Metallurgy) A-1
ANL(SS) D
Armour Res Foundation(Elliott) AT(11-1)-578 #19
Cal U(Berk)(Portis) AT(04-3)-34 Proj No 47
Cal(Riv)(Lawson) AT(11-1)-34 #77
Den U(Nachman/Lundin)
Ill U(Maurer) II B AT(11-1)-1198
NBS(Brower) 0905-11-09450
Penn St(Gingerich) AT(30-1)-2541
Pitts Univ of(Wallace) AT(30-1)-647
Pitts Univ of(Craig) AT(30-1)-2163
RPI(Burr) AT(30-1)-2159
RPI(Greene) AT(30-1)-2714
Union Carbide(Met) D-3
VPI(Leinhardt)
West Virginia Univ(Pavlovic) AT(40-1)-2839
WRU(Major) AT(11-1)-1146

Recovery and Recrystallization
ANL(Met) F-1
Calif U of(LRL)(Berkeley) A-2
Hanford Atomic Products Operation(Pu) AT(30-1)-1350
Ill U(Maurer) III E
Penn U(Brown) AT(30-1)-1893
Union Carbide Nuclear Co(Met) B-2, -4
Utah(Cutler) AT(11-1)-1122

Refractories - See Ceramics and Refractories - Refractory Metals - See Body-centered cubic metals

Rhenium, pure, alloys, compounds
California(LRL) C
Ill U of(Maurer) II A

S

Semiconductors, elements and compounds
Ames, SS dw 3, 5
ANL(SS) B-3b; C-2; Eb
Arizona State(Gossick) AT(11-1)-715 A I - C
Brown U(Bray/Hooper) AT(30-1)-2024
Chicago Univ of(Rice) AT(11-1)-357
Cinci U(Hoch/Meeks) AT(11-1)-1115
Illinois Univ of(Maurer) III F AT(11-1)-1198
JHU(Bearden) AT(30-1)-2185 and -2543
Louisiana State(Reynolds) AT(40-1)-3087
NBS(Frederikse) #13443
Northwestern Univ(Kauffman) AT(11-1)-1161
Penn State(Bell)
Pa Univ of(Burstein) AT(30-1)-2395
Princeton(Smoluchowski) AT(30-1)-2680
Purdue Univ(James) AT(11-1)-125
Stanf(Macres/Huggins) AT(30-1)-298
Tenn U(Stansbury) AT(40-1)-1068
Union Carbide Corp(Westbrook) AT(30-1)-2051
Union Carbide Nuclear Co(SS) A-3; B
Va Univ of(Catlin) AT(40-1)-3012

Silica
ANL(SS) C-2
BNL(SS) A-1
MIT(King) AT(30-1)-1985
North Dakota(Bale) AT(11-1)-1255
U C(SS) D-4

Single Crystal Preparation
ANL(Met) A-4
Brn U(Bray) AT(30-1)-2024
Cath U(Meijer) AT(40-1)-2861
CIT(Vreeland/Wood) AT(04-3)-473
Chi U(Rice) AT(11-1)-357
Cornell U(Silsbee/Bowers) AT(30-1)-2150
Cornell Univ(Webb/Silcox) #3029
HAPO(Pu)
Illinois(Simmons) AT(11-1)-1198
MRC(Abowitz) AT(30-1)-2980
NBS(Brower) 0905-11-09450
Union Carbide Corp(Westbrook) AT(30-1)-2051
Union Carbide Nuclear Co(Met) A-1
Union Carbide Nuclear Co(SS) C-1
VISR(Kirn) AT(40-1)-2860
Yale(Wolf)

Sintering
Calif U of(Berkeley) B-3
Florida Univ of(Rhines) AT(40-1)-2581
Ill U(Maurer) IV D AT(11-1)-1198
MIT(Kingery) AT(30-1)-2574
RPI(Lenel) AT(30-1)-2408
Union Carbide Nuclear Co(Met) C-1
Utah Univ of(Cutler) AT(11-1)-1122

Solid State Theory, Calculations of Structure, properties, and behavior from models and first principles
ANL(SS) E-a, b, c, d, e, f
BNL(SS) A-4a, b
Case(Smith) AT(11-1)-623
C U(Sproull/Krumhansl) AT(30-1)-2391
Del U(Skolnick) AT(30-1)-2722
Ill U(Maurer) II C AT(11-1)-1198
Kansas Univ of(Friauf)
MIT(Averbach/Cohen) AT(30-1)-2879
MSU(Blatt) AT(11-1)-1247
Princeton Univ(Smoluchowski) AT(30-1)-2680
RPI(Brown) AT(30-1)-1995
Temple(Muldawer/Amar) AT(30-1)-2812
Tufts(Handler) AT(30-1)-2968
Union Carbide Co(SS) A-1, -2, -3, -4
VPI(Leinhardt) AT(40-1)-2689

Solidification - See Melting and Solidification

Sputtering
General Mills(Wehner) AT(11-1)-722
Houston Univ of(Reynolds/Allred) AT(40-1)-2573
Union Carbide Nuclear Co(SS) A-2; C-4

Stacking faults - defects in crystalline solids

Substitutional Solid Solution, Structure and Properties
Ames(Met) B-1, -2, -3
Ames(SS) 1
ANL(Met) A-2; B-1, -2, -3, -4, -6, -8; D-4, -5
ANL(SS) B-3a
Ariz U(Murphy) AT(11-1)-1040
A I - A
BNL(Met) B-1
Calif(LRL) A-1
Cinci U(Hoch/Meeks) AT(11-1)-1115
Del U(Skolnick) AT(30-1)-2722
Denver Univ of(Colorado Seminary) (Nachman/Lundin)
Fla U(Guy) AT(40-1)-2857
Ill U(Maurer) II E AT(11-1)-1198
IBM(Nowick) AT(30-1)-2811
MIT(Averbach/Cohen) AT(30-1)-2879
MIT(Warren) AT(30-1)-3020
Mich Coll of Mining and Tech (Hendrickson)
Minnesota Univ of(Nicholson) AT(11-1)-1009
Mississippi Univ of(Lewis) AT(40-1)-2891
RPI(Huntington) AT(30-1)-1044
Temple Univ(Muldawer/Amar) AT(30-1)-2812
Tennessee Univ of(Stansbury) AT(40-1)-1068
U C(Met) B-1, -3, -4; D-3
Vblt(Wert) AT(40-1)-3091
Wake Forest College(Turner) AT(40-1)-2413
WRU(Greene)
Wisconsin Univ of(Dodd)

Sulfides - See Phosphides and Sulfides

Superconductivity
Ames, SS dw 1, 2
ANL(Met) B-8
A I - A
Cal Tech(Duwez) AT(04-3)-221
Cal U(Berk)(Portis) AT(11-1)-34 Proj No 47
Calif Univ of(Dransfeld) AT(11-1)-34 #76
Calif U of(Lawson) AT(11-1)-34 #77
Chicago Univ of(Rice) AT(11-1)-357
Cornell Univ(Webb/Silcox) #3029
MIT(Pearsall)
Pa Univ of(Burstein) AT(30-1)-2395
Union Carbide Nuclear Co(Met) B-1, -3
Union Carbide Nuclear Co(SS) C-5
VPI(Leinhardt) AT(40-1)-2689

Surface reactions - See Corrosion

Surfaces and thin films, structure and physical properties of
ANL(Met) F-2, -3
A I - C
BNL(Met) B-2
Cal Tech(Duwez) AT(04-3)-221
Carnegie I T(Shewmon) AT(30-1)-2314
Case(Smith) AT(11-1)-623
Chi U(Rice) AT(11-1)-357
Cornell(Silcox/Webb)
Cornell Univ(Che-Yu Li) AT(30-1)-3228
Franklin Inst(Wilsdorf) AT(30-1)-2994
Georgia Inst(Scheibner) AT(40-1)-2755
Ill U(Maurer) III C, D, F
Little, Arthur D Inc(Davis) AT(30-1)-2756
MSU(Blatt) AT(11-1)-1247

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PRINCIPAL INVESTIGATOR INDEX

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SUBJECT INDEX