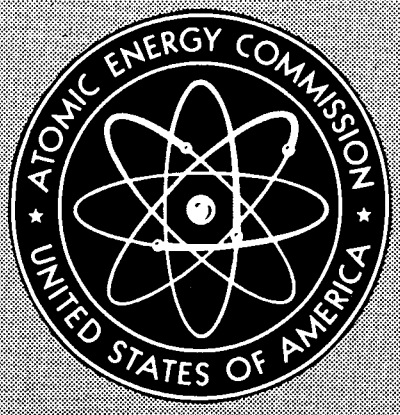

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METALS, CERAMICS, AND MATERIALS

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

Edited by
R. J. Allio

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Division of Research, AEC
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UNITED STATES ATOMIC ENERGY COMMISSION • OFFICE OF TECHNICAL INFORMATION

USAEC Office of Technical Information Extension
Oak Ridge, Tennessee

FOREWORD

In addition to conducting scientific research in its own laboratories, the Atomic Energy Commission provides assistance to universities, research institutes, independent laboratories, industrial laboratories, and other government agencies who can contribute to the research program of the Commission. Such assistance takes the form of financial support for payment of salaries, purchase of equipment and other materials, and allowance for overhead costs and is formalized by direct contract between the Commission and the organization performing the work. Both basic and applied research studied are involved.

Under these contractual arrangements, physical research is being performed in metallurgy, chemistry, and physics. For each of the fields of science, summaries of the physical research projects under way at the various sites are published from time to time as directories. These directories serve to assist researchers in exchanging ideas and to acquaint them with related programs at other laboratories.

This document summarizes the objectives and current status of the individual research projects supported by the Metallurgy and Materials Branch, Division of Research, in the fields of physical metallurgy, solid state physics and physical ceramics. It includes the research conducted at the Commission's laboratories as well as that performed at university and other laboratories. These summaries were prepared primarily by the investigators whose names appear on the summary sheets.

The information has been organized into three broad categories:

I. Production Treatment and Properties of Materials
II. Physical Research in the Nature of Matter
III. Interaction of Radiation with Matter

Two indexes appear at the end of the directory, one arranged by subject and another arranged alphabetically by contractor.

All of the research presented in this document is unclassified. As a normal procedure, periodic progress reports of information resulting from these contracts are not prepared. Investigators are urged to report their results in the open literature at the earliest opportunity for wide dissemination of the information.

Section I

PRODUCTION, TREATMENT, AND PROPERTIES OF MATERIALS

I-A

Materials Preparation

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

Contract: W-7405-eng-82

Brief Title: HIGH PURITY METALS RESEARCH

Investigators: O. N. Carlson, A. H. Daane, D. T. Peterson, F. H. Spedding, and H. A. Wilhelm

Scope of Work

Experimental results on the behavior of metals and alloys depend upon the purity of the materials used. Because many metals are not available commercially in the purity desired, considerable effort is devoted toward the preparation of metals of high purity. The iodide crystal bar technique, zone refining, distillation, sublimation, calcium treatment, electron beam melting, vacuum annealing and other means are being employed in studies on the preparation of some pure metals.

High vacuum distillation has been very effective in improving the purity of the more volatile rare earths and this technique is being extended to some of the less volatile materials by devising improved furnaces. Crystal bar techniques are being employed on vanadium, thorium and niobium. The crystal bar preparation of vanadium gives good quality metal on a relatively large scale. Further improvement in the quality of this metal has been obtained, however, by the calcium bath treatment.

The preparation of pure metals by carbon reduction of oxides offers possibilities in some cases. High purity carbon mixed with a suitable high purity oxide can give a metal that has low impurity content. This method is being studied as a means for the preparation of metals such as niobium, tantalum and uranium.

Contractor: Anderson Physical Laboratory, Champaign, Illinois

Contract: AT(11-1)-544

Brief Title: PURIFICATION OF ALKALI HALIDES

Investigators: Scott Anderson

Scope of Work

The objective of the proposed effort is to produce in reasonable quantity ultra high purity potassium chloride and potassium bromide together with detailed chemical analyses of each lot of salt. In addition, it is further intended to develop proper procedures and techniques leading to the production and analysis of ultra high purity sodium chloride and sodium bromide.

Contractor: Battelle Memorial Institute, Columbus, Ohio

Contract: W-7405-eng-92

Brief Title: GROWTH OF SINGLE CRYSTALS OF UO_2

Investigators: F. A. Rough

Scope of Work

The objective of the program on UO_2 crystal growth is to develop methods and techniques for growing single crystals of high purity and of sufficient size for studies of transport properties of UO_2. X-ray, optical, and electrical measurements conducted on stoichiometric UO_2 crystals and on crystals with slight excess of oxygen (UO_{2+x}) would provide information needed to elucidate the nature (structure, purity, crystal perfection, kind and concentration of charge carriers) of UO_2. The present study is concentrated on the growth of UO_2 crystals by fusion techniques. Loss of UO_2 by volatilization at the temperature of fusion must be minimized by providing an ambient cover of inert gas or by conducting the experiments in sealed or capped tungsten containers. Several sources providing the energy for melting are being investigated. These include resistance heating of tungsten, induction heating, electron beam melting, arc melting, and plasma jet impingement. Crystal growth has been accomplished by directional solidification of the melt, in particular by the Bridgman drop method. Possibilities of zone melting and of use of Czochralski pulling techniques have also been considered.

Contractor: Michigan State University, East Lansing, Michigan

Contract:

Brief Title: GROWTH AND PROPERTIES OF METAL AND COMPOUND SINGLE CRYSTALS

Investigators: William E. Taylor

Scope of Work

This program deals with the production of crystals which are either free from dislocation or which have closely controlled dislocation concentrations. The research includes the following phases of work:

(a) Growth of crystals of Zn under controlled thermal gradients to minimize dislocation formation. Techniques may be extended subsequently to other materials.

(b) Development of etch pit technique for determination of dislocation density.

(c) Correlation of etch pit studies with x-ray data obtained by the Lang or Newkirk method.

(d) Analysis of dislocation interaction in crystals after varying amounts of plastic deformation.

Contractor: National Bureau of Standards, Washington, D.C.

Contract: NBS Project No. 09450

Brief Title: CRYSTAL GROWTH

Investigators: W. S. Brower and A. D. Franklin

Scope of Work

The objective of this program is the study of the influence of the atmosphere on the crystalline perfection of crystals such as TiO_2, ferrites, titanates, and other high melting substances as grown by the Verneuil technique. Techniques will be developed for growing such crystals with control over the impurity and defect population.

Contractor: Parma Research Laboratory of Union Carbide Corporation
Cleveland, Ohio

Contract: AT(30-1)-2051

Brief Title: HIGH QUALITY SEMICONDUCTOR MATERIALS

Investigators: R. D. Westbrook, R. L. Cummerow

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: Union Carbide Nuclear Company, Oak Ridge National Laboratory
Oak Ridge, Tennessee

Contract: W-7405-eng-26

Brief Title: PREPARATION OF RESEARCH MATERIALS

Investigators: C. T. Butler, J. H. Crawford, Jr., and C. C. Robinson

Scope of Work

It is well known that one of the main limitations to progress in investigations of solids is the lack of availability of material of either high purity or controlled impurity content. The rapid progress over the past decade in elemental semiconductors was made possible by the perfection of research specimen preparation techniques. The research program in question is devoted to the development of techniques for both the production and quality evaluation of certain crystals of importance to fundamental investigations of solids. At the present time those materials under consideration are: isotopically pure Li^6 and Li^7 fluoride; refractory body-centered cubic metals, potassium chloride crystals of high structural perfection (low dislocation density) as well as specimens of carefully controlled impurity content, single crystals of Cu O of known stoichiometry, and high purity MgO crystals. Some success has already been achieved with the lithium fluoride and Cu_2O. It is hoped that additional materials can be considered in the future. Methods of evaluation include optical and magnetic investigations, x-ray structure determination, and both spectrographic and activation microanalysis.

Contractor: Union Carbide Nuclear Company, Oak Ridge National Laboratory
Oak Ridge, Tennessee

Contract: W-7405-eng-26

Brief Title: CRYSTAL PHYSICS

Investigators: G. W. Clark and C. B. Finch

Scope of Work

This is a program for studying growth processes of crystals of high-temperature materials. A better understanding of growth mechanisms, and influences, such as impurities and system parameters, is desired. A very important product is acquiring the know-how and growing quality mono-crystals of known perfection, composition, and purity. The materials studied are of current fundamental interest or are suited for the testing of concepts.

The facilities are to 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 d.c. arc plasma torch and a r.f. 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.

More specifically, studies are in progress on the growth of Fe_3O_4 and MgO hydrothermally. Work has been initiated to determine the characteristics of solutions demonstrating good solvent and transport action in supercritical systems. Crystallization kinetics of materials from supersaturated melts are being investigated as a function of temperature and degree of supersaturation. For the flame fusion process, the effort is to define the critical parameters and determine their effect on the growth process and crystal quality. Both the d.c. arc and r.f. inductively coupled plasmas are being engineered as controlled heat sources for the flame fusion process.

Section I-B

Sintering and Solidification

Contractor: Argonne National Laboratory, Lemont, Illinois

Contract: W31-109-eng-38

Brief Title: PHYSICAL CERAMICS

Investigators: A. Arenberg, C. Araoz, P. Stablein, M. Volpe

Scope of Work

The objectives in this area have been to determine the mechanisms of atom mobility in oxides and to study the effects of deviations from stoichiometry and imperfections on these processes. Studies on Al_2O_3 single crystals have shown that although the mechanism of sintering in both oxidizing and reducing atmospheres is the same, namely volume diffusion, the rates of diffusion are appreciably different, due to differences in the kind of imperfections produced on the surfaces.

The same experimental technique that was used on Al_2O_3 spheres was applied to the study of sintering in UO_2, but to date without much success because of high evaporation rates. In view of this, current efforts are directed toward measuring O_2 diffusion rates as a function of oxygen excess, and to correlate these with the effects of oxygen excess on sintering.

Another program currently initiated deals with studies on the effects of crystalline structure on electron emission from both metallic and non-metallic surfaces, using field emission microscopy techniques.

Contractor: Cornell University, Ithaca, New York

Contract: AT(30-1)-2558

Brief Title: SOLIDIFICATION REACTIONS

Investigators: Harry W. Weart

Scope of Work

It is the purpose of this project to study the origin and characteristics of a subgrain structure, the colony structure, that is formed during solidification of binary eutectic alloys. This structure is of interest because its existence reveals the inadequacy of the classical concept of eutectic solidification, which envisions only short-range concentration gradients in the liquid, parallel to the solid-liquid interface. In addition to these gradients, which partition the major components of the liquid to form the constituent phases of the solid eutectic, long-range gradients, which are perpendicular to the interface, also exist in the liquid. These latter gradients appear to be an essential cause of the cellular topography of the solid-liquid interface, whose motion is known to produce the colony structure. This project will concern itself with identifying the source of the long-range concentration gradients and with examining the manner in which these gradients affect the colony structure through their interaction with growth parameters.

Identification of the source of the concentration gradients will be attempted by using zone-melting to measure the partition coefficients both of major components and of representative impurities between the solidifying eutectic and its melt. The response of the dimensions of individual phase particles and of colonies to controlled alterations of growth parameters will also be studied. Such information is expected to permit some deductions concerning the details of the component redistribution that accompanies eutectic solidification.

Contractor: Florida, University of, Gainesville, Florida

Contract: AT(40-1)-2581

Brief Title: TOPOLOGICAL STUDY OF THE SINTERING PROCESS

Investigators: Frederick N. Rhines and John Kronsbein

Scope of Work

In order to prove that surface tension provides the primary driving force of sintering, measurements are being made of the tensile force that is required to stop sintering contraction. A phenomenological theory has been developed to relate the sintering force to the average specific interfacial free energy (γ) of the sintering material through certain geometric parameters.

A new test of the Herring analysis of material transport during sintering is based upon the topological deduction that neck growth results simultaneously or alternatively from two independent geometric processes, namely, (1) surface rounding and (2) a decrease in the distance between particle centers. These geometric factors are being separated for study by using a series of particle sizes in the Kuczynski experiment and extrapolating the rates of neck growth to the conditions of (a) very small particle diameter and (b) very large particle diameter. In case (a) the effect of the approach of particle center should be magnified, while in case (b) surface rounding should predominate. It is thought that different rates of material transport may apply to the two cases.

Indications from earlier studies, by the authors, that there is a direct relationship in sintering between the density and the internal surface area, is being subjected to more detailed scrutiny, in order to ascertain how general may be the relationship and in order to discover its cause.

Contractor: (The) Franklin Institute Laboratories for Research and Development, Philadelphia, Pennsylvania

Contract: AT(30-1)-2503

Brief Title: RESEARCH ON FUNDAMENTAL CONSIDERATIONS IN SINTERING

Investigators: M. Herman

Scope of Work

The theories of sintering which have been derived to quantitatively describe the mass transport of material by diffusion are applicable principally during the early stages where the changes in geometry can be related in a simple manner to the volume of material transported. While there are numerous investigations dealing essentially with single asperity bonds, there is very limited information on the early stage sintering of aggregates of fine metal particles in which the changes in geometry have been accurately measured. In the present investigation the experimental difficulty of determining the early stage change in geometry in powder compacts has been overcome by measuring the continuous densification of loosely packed aggregates of fine metal particles as the temperature of the system is slowly but uniformly increased. A mathematical method based upon diffusion theories of sintering has been derived to treat this geometrical change under the non-isothermal conditions so that the time dependence, size dependence, activation energies, and diffusion coefficients obtained can be used to determine the details of the mass transport mechanisms.

Contractor: General Telephone & Electronics Labs., Bayside, New York

Contract: AT(30-1)-GEN-366

Brief Title: FUNDAMENTALS OF SINTERING AND BONDING

Investigators: L. L. Seigle, L. Castleman, J. Brett and M. Nicholas

Scope of Work

Research under this contract is carried out in the two areas described below:

Fundamentals of Sintering of Metals and Oxides

The objective of this project is to clarify the structural factors and mass transport processes which underlie bond formation between particles and densification of powder compacts, both metal and oxide. One phase of the project is concerned with the influence of grain boundaries and grain boundary impurities upon rates of sintering. Another phase is devoted to clarifying the mechanisms controlling the initial stages of bonding during compaction of powders.

Experiments are being performed to evaluate the influence of impurities and atmospheres on the activity of grain boundary vacancy sinks during sintering in a variety of metal powders. The migration of vacancies in the vicinity of grain boundaries is being studied through an exploration of the geometry of grain boundary grooves in model wire compacts. Changes in the distribution and frequency of dislocations in the vicinity of grain boundaries in such compacts are being followed through use of etch pit techniques.

In studies of the bonding of metal particles under pressure, the relationships between load, relative shear, and bond strength are being determined for metal surfaces pressed and twisted together at room and elevated temperatures. The influence of surface condition upon bond strength is being investigated and the effect of surface active agents. Time and temperature effects are being studied in order to clarify the mechanisms underlying the initiation and strength of interparticle bonds.

Fundamentals of Diffusional Bonding

The objective of this project is to clarify the processes affecting the growth at elevated temperatures of intermetallic layers which nucleate at the bonded interface between two dissimilar metals. A knowledge of the factors affecting the kinetics of such processes is of considerable importance to fuel element technology, since practically all metallic fuel elements are bonded structures, and it has been empirically determined that bond properties deteriorate as intermetallic layers grow. The scope of the program includes an

evaluation in interdiffusing multi-phase metallic systems of the factors which affect the motion of phase interfaces and the growth of the intermetallic layers. Such factors include the following: the effects of temperature, time, and applied pressure; the effects of the atomic arrangements within the intermetallic layers, such as the state of order; and the effects of mutually interfering diffusion or other currents. The analysis of the experimental results is based on the available phenomenological multi-phase diffusion theory and on pertinent theoretical models; the effects of pressure are considered in terms of its influence both on the thermodynamics of the system and the kinetics of the interdiffusion processes. As part of the program, work has been completed on the study of intermetallic layer growth in the Ni-Al, U-Al, and Th-Al systems, and an investigation is currently under way on the growth in the Cu-Zn system of beta brass layers in the ordered and disordered states.

Contractor: Harvard University, Cambridge, Massachusetts

Contract: AT(30-1) 2305

Brief Title: A STUDY OF NUCLEATION AND GROWTH OF CRYSTALS IN SUPERCOOLED LIQUIDS

Investigators: Bruce Chalmers

Scope of Work

Measurements have been made of the growth rate of dendrites in supercooled water and dilute aqueous solutions. Similar measurements have been made in lead-tin alloys. Growth rate measurements also have been made for growth of dendrites along various substrates. The morphology of the non-crystallographic dendrites which grow in aqueous solutions has been studied. These measurements and studies contribute considerably to our knowledge of growth of dendrites in supercooled liquids.

Nucleation phenomena in supercooled water are currently under investigation. The study of growth in supercooled liquids and alloys will be continued.

Contractor: Harvard University, Cambridge, Massachusetts

Contract: AT(30-1)-1956

Brief 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: Illinois, University of, Urbana, Illinois

Contract: AT(11-1)-915

Brief Title: CRYSTALLIZATION OF PEROVSKITE LEAD TITANATE FROM GLASSES

Investigators: A. L. Friedberg and C. G. Bergeron

Scope of Work

Ferroelectric compounds of the perovskite structural type such as barium titanate, lead titanate, and potassium niobate have been investigated extensively in single crystal and polycrystalline form. Little information has been reported concerning the nucleation and crystal growth of such phases from glasses, or about the crystal formation and growth behavior of crystallizing glass systems in the presence of static external electric fields.

The proposed research project is concerned with a study of the crystallization of lead titanate from glasses in the systems $PbO.TiO_2.SiO_2.Al_2O_3$ and $PbO.TiO_2.B_2O_3$. It is proposed to study the relationship between the rate of nucleation and crystal growth of lead titanate from glasses as a function of the temperature and viscosity of the melt, and to study the size, spatial orientation, tetragonal distortion, and electric state of the lead titanate crystals formed from these glasses.

An additional objective is to study further these relationships of the resulting crystals as a function of the intensity and direction of an electric field applied during crystallization. Studies made both above and below the Curie temperature for lead titanate ($490^{\circ}C.$) are expected to show whether the interaction between the spontaneous dipole moment and the applied field is of sufficient magnitude to cause preferential orientation in space of the polar axis of the resulting crystals.

Contractor: Rensselaer Polytechnic Institute, Troy, New York

Contract: AT(30-1)-2408

Brief Title: MECHANISM OF SINTERING LOOSE AND PRESSED METAL POWDER COMPACTS

Investigators: Fritz V. Lenel

Scope of Work

This project is concerned with a study of the sintering behavior of loose metal powder aggregates and metal powder compacts. In the first phase of the project the relative shrinkage in the radial and in the axial directions of both conventionally pressed copper powder compacts and of loose copper powder aggregates was determined. The results of the experimental work led to the tentative conclusion that the theories previously advanced to explain the differences in the axial and radial shrinkage of compacts and aggregates are not correct. The pores of green and sintered compacts of irregular copper powder are not necessarily disk or lens shaped, but rather equiaxed and the observed difference in shrinkage cannot be attributed to the shape of the pores. On the other hand, the ratio of axial and radial shrinkage of irregular shaped powder and of flake powder aggregates is nearly the same in spite of the fact that the pores in the flake powder aggregates are much larger in the radial than in the axial direction.

On the basis of the experiments described it was concluded that the action of surface tension forces cannot adequately explain the observed ratios of radial and axial shrinkage in either compacts or loose powder aggregates. It was tentatively postulated that gravity is responsible for the observed ratio of shrinkage in loose powder aggregates while residual stresses are responsible for the observed shrinkage effects in compacts with interconnecting pores.

In the second phase of the project the effect of residual stresses on the shrinkage behavior of compacts is studied. In the third phase of the project changes in the electrical resistance of loose powder aggregates are studied, when the aggregates are sintered at low temperatures. These changes should indicated changes in the contact area between particles and may lead to a better understanding of the mechanism of atom movement during sintering at these temperatures.

Contractor: Utah, University of, Salt Lake City, Utah

Contract: AT(11-1)-82, Proj. No. 9

Brief Title: RECRYSTALLIZATION AND SINTERING OF OXIDES

Investigators: Ivan B. Cutler

Scope of Work

Ceramic materials have generally been so grossly impure that little attention has been paid to the influence of minor amounts of impurities. This project is designed to study impurities as they influence crystal imperfections and alter chemical and physical properties of ceramic materials. Five individual problems are proposed for study as part of this project.

The first problem concerns the kinetics of shrinkage of compacts of oxide powders during sintering. According to theory, the rate of shrinkage of powders compacts may be related to the diffusion of lattice vacancies. This problem is an investigation of the validity of the theory and also its relationship to non-stoichiometry built into the lattice through addition of certain impurities.

Another problem is an investigation of the electrical conductivity of single and polycrystalline alumina. The wide divergence of results reported in the literature suggests the importance of impurities in the conduction process. To date it has been possible to show that experimental techniques are at least partially responsible for the variations in reported conductivities.

Growth of single crystals in polycrystalline compacts of alumina illustrates the exaggerated grain growth so characteristic of sintered alumina. The mechanism of growth is not understood. It appears to be very sensitive to the presence of impurities. In this problem, the mechanism of growth will be studied.

The problem of the kinetics of diffusion of impurities into crystals of alumina and magnesia appears to be experimentally feasible through the observation of the movement of an interface between the diffused portion and undiffused part of the crystals. Colored ions such as iron ions make this interface visible. Measurements of diffusion will be made by following the rate of movement of the interface.

Grain growth in sintered magnesia and sintered calcia follows the simple grain growth laws developed for metals. The problem at hand is an experimental study of the rate of grain growth as it is related to the impurity content. In particular, impurities will be studied that alter the concentration of vacancies and the diffusion constant.

Section I-C

Thermodynamics, Transformations and Phase Equilibria

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

Contract: W-7405-eng-82

Brief Title: PHASE EQUILIBRIA AND THERMODYNAMIC PROPERTIES

Investigators: P. Chiotti, W. L. Larsen, J. F. Smith and F. H. Spedding

Scope of Work

A knowledge of phase equilibria and a knowledge of thermodynamic properties are both important in predicting the behavior of metals and alloys. For many purposes this information is much more meaningful than a tabulation of empirical data.

Thermodynamic functions of some intermetallic compounds are determined from vapor pressure of a metal from a binary system. Work on binary magnesium alloys with calcium, copper, nickel and yttrium give compound heat of formation data that are in agreement with that by other methods where such other data are available.

Phase relationships for many binary alloy systems are being investigated. In the aluminum-tantalum system, for example, compounds Al_3Ta, $AlTa_2$ and possibly $AlTa_3$ are believed to exist. Characterization of these compounds and determination of some properties of the alloys are a part of the study. Similar investigations are being made on alloys of Bi-Zr, Nb-Sn, Nb-Al, Ta-Zr, Th-Ta, Ni-Zr, Ni-Hf, Co-Zr, U-Re, Nb-Zr-O, Y-Zn, Cr-Re, Y-O, Ca-CaH_2, Sr-SrH_2, Mg-Y, Zr-C-H_2, Hf-C-H_2, Ti-C-H_2, Y-C-H_2, Pb-Zn-Sn, Pb-Zn-Th.

Contractor: Argonne National Laboratory, Lemont, Illinois

Contract: W31-109-eng-38

Brief Title: URANIUM AND PLUTONIUM CONSTITUTION DIAGRAMS

Investigators: A. F. Berndt, A. E. Dwight, D. B. Jugle, M. B. Nevitt, S. Rosen, S. T. Zegler

Scope of Work

Scope I. Uranium Diagrams

Work on binary and ternary phase diagrams in which U is the only 5f metal involved is in its final stage. A brief summary can be made as follows:

U-C: Determination of liquid-solid equilibrium relations at low carbon content is complete. No further work is in progress.

U-Zr: A reinvestigation of certain conflicting features of earlier versions of the diagram has been completed. No further work is in progress.

U-Zr-Nb and U-Nb: Work on the ternary system U-Zr-Nb was terminated upon establishment of the phase relations in the U-rich corner below the solidus. The study of the U-Nb binary system was made in conjunction with the ternary diagram work and has also been completed. The kinetics of solid phase transformations in U-Zr-Nb alloys have also been studied.

U-Mo: The diagram up to 19 w/o Mo and below 900°C has been determined. Two important differences between this diagram and earlier versions are: (a) The delta phase is believed to form congruently rather than by a peritectoid reaction. (b) The temperature of the eutectoid transformation $\beta \rightarrow \alpha + \gamma$ was found to be 639°C, which is lower than reported by earlier investigators.

U-Ru: Experimental work on the region below the solidus in this system is essentially complete. The system is characterized by moderately high solubility of Ru in gamma U and by the occurrence of six intermetallic compounds. The structure of U_2Ru has been identified.

U-Rh: The study of this system, which was limited to the composition range from 0 to 33 atomic pct Rh, has now ended. Within this limited composition range the system has a close resemblance to U-Ru.

U-Ru-Mo: The study of the U-rich corner of this ternary system is still underway. The phase relations at high temperature are dominated by a large gamma phase field and the compound U_2Ru.

Scope II Diagrams Involving Plutonium

The effort in this area is centered in studies of three ternary systems involving Pu. In two of the systems U is one of the other components.

U-Pu-C: This investigation is concerned with phase relations below the solidus and in the composition range below 50 atomic pct carbon.

U-Pu-Ru: The essential features of a limited number of isothermal sections below the solidus are being studied.

Pu-Ru-Mo: The phase relations in the Pu-rich corner of this system are of concern in this portion of the program.

Substantial progress has been made on the U-Pu-C system. Work on the other two systems is in an early stage.

Contractor: California, University of, Berkeley, California

Contract: AT(11-1)-34, Proj. No. 33

Brief Title: THERMODYNAMIC FUNCTIONS FOR THE METALLIC STATE

Investigators: R. R. Hultgren

Scope of Work

The purpose of this program is the critical examination of all published experimental data on the field of thermodynamics of metals and binary alloys. Each publication is checked for internal consistency, for agreement with other works, with the phase diagram, and with other properties of the system. For each system a set of the most probable values of thermodynamic functions is compiled giving reasons for the choices in a short, critical discussion. Where possible, probable limits of error on each value are assigned. The results are published in loose-leaf multilith form and the sheets are sent when completed to all laboratories which request them. During the summer of 1961 it is expected to complete the survey of all metallic systems and to publish the work in book form. After this, revisions will be continuously made and issued as loose-leaf sheets in order to keep the data up to date.

Contractor: Case Institute of Technology, Cleveland, Ohio

Contract: AT(11-1)-588

Brief Title: TRANSFORMATION CHARACTERISTICS OF ZIRCONIUM-NIOBIUM ALLOYS

Investigators: Robert F. Hehemann

Scope of Work

Transformations in Zr-Nb alloys are extremely varied and encompass virtually all of the recognized transformation mechanisms. Hypermonotectoid alloys are particularly interesting. Although cellular or pearlitic microstructures might be expected from the eutectoidal nature of this system, these structures have been observed at temperatures above as well as below the monotectoid temperature. This is particularly significant in regard to the several theoretical treatments of this decomposition mechanism which have appeared in the literature. Transformation kinetics in the hypermonotectoid range will be examined systematically in order to explore the range of validity of these several theoretical models.

The problems connected with the omega reaction which occurs on aging at lower temperatures have been crystallized considerably during the past year. Single crystal x-ray diffraction studies offer promise of establishing the relationship between the purely crystallographic and the imperfection descriptions of the structure which have evolved in the literature. This may lead to a physical interpretation of the decomposition mechanism.

Study of transport properties (at present electical conductivity) offers promise of establishing a connection between the structural characteristics of this transformation and the associated changes in physical properties. Initial efforts along these lines will be directed toward achieving a better understanding of the negative temperature coefficient of resistivity which has been observed in quenched alloys.

Contractor: Illinois, University of, Urbana, Illinois

Contract: AT(11-1)-67 Proj. No. 15

Brief Title: DIFFUSIONLESS PHASE CHANGES IN NON-FERROUS METALS AND ALLOYS

Investigators: T. A. Read and D. S. Lieberman

Scope of Work

It is planned to complete the calorimetric determination of work on the latent heat of transformation on the 47.5 atomic pct. Cd alloy and begin studies of the two distinctly different transformations in the 49 pct. Cd alloy. The radio-active tracer diffusion investigations should be completed on one set of AuCd alloys during the next contractual period and extended to other compositions and the AuZn system. X-ray and resistivity measurements on both of these systems (including both attemperature and studies of quenched specimens) will be extended to determine whether these alloys possess defect structures and to ascertain the state of order as affected by composition, previous history, etc.

Transmission electron microscopy studies will be undertaken to determine the nature of the interface in the AuCd alloy transformations as well as the types of dislocation arrays involved in the "rubber-like" behavior. The transformation in the vanadium-ruthenium systems of equatomic composition was observed by resistivity measurements and resembles those involving changes in magnetization; x-ray structure determinations of the two phases will be made and magnetic investigations will be initiated. Efforts will also be made to study the crystallography of the transformations in at least two other systems, manganese-bismuth and silver selenide.

Contractor: Massachusetts Institute of Technology, Cambridge, Massachusetts

Contract: AT(30-1)-1002, Scope II

Brief Title: THERMODYNAMICS AND STRUCTURE OF SOLID SOLUTIONS

Investigators: B. L. Averbach and Morris Cohen

Scope of Work

X-ray diffraction and thermodynamic methods are being used to investigate the fundamental atomic arrangements and bonding mechanisms in solid solutions. During the past year, measurements of the relative thermodynamic properties of the iron-aluminum system were completed and a technical report has been submitted for publication. X-ray and thermodynamic measurements are now being undertaken on iron-silicon alloys. A Monte Carlo calculation of the short-range order is also being made using an IBM 709 computer.

Contractor: Massachusetts Institute of Technology, Cambridge, Mass.

Contract: AT(30-1)-1002, Scope I

Brief Title: THERMODYNAMIC AND OTHER PROPERTIES OF METALLIC SYSTEMS

Investigators: Michael B. Bever

Scope of Work

This research is concerned with (1) the effects of deformation and annealing on the properties of metals, in particular the stored energy of cold work and (2) the thermochemistry of alloy systems. A liquid metal solution calorimeter is used for measuring heats of formation, heats of solution and other energy effects. A constant-temperature gradient calorimeter is now available for measuring heat capacities and heat effects of phase changes.

(1) Deformation and Annealing - The following variables affecting the stored energy of cold work have been investigated: the deformation process (including explosive deformation), the strain, the strain rate, the temperature of deformation (R.T.. 78°K and 4°K in an exploratory investigation) and the composition (Au, Ag and Au-Ag alloys; ordered and disordered Cu_3Au). Changes in the stored energy have been related to changes in the structure, the mechanical properties, and the resistivity.

The effects of annealing of cold-worked metals are being investigated. The hardness and stored energy of polycrystalline gold-silver alloys worked successively at 78°K and R.T. have been found to show the work softening effect, which sheds some light on the imperfections generated by deformation at low temperatures.

Current work is concerned with deformation of gold at 78°K and at R.T. The kinetics of annealing after deformation below room temperature are also being investigated.

(2) Thermochemistry of Alloys - The heats of solution in tin of elements in Groups IB and IIIB and of other elements have been measured. Bismuth and tin-bismuth alloys as solvents have also been investigated.

Heats of formation of solid solutions in the gold-silver, copper-tin and copper-nickel systems and the heats of formation of Cu_3Au and the III-V compounds, InAs, InSb, and GaSb have been measured. An investigation of the heats of formation of all intermediate phases in the gold-tin system has recently been completed. Other investigations have been concerned with the energy of ordering in Cu_3Au, the energy of precipitation of Cu_3Sn from alpha Cu-Sn and the excess energy in electrodeposited silver.

The measurement of heats of solution and heats of formation is being continued in order to obtain thermodynamic data of interest and to gain some insight into the bonding of the alloys investigated.

Contractor: National Bureau of Standards, Washington, D.C.

Contract: NBS Project No. 0802-11-08420

Brief Title: CONSTITUTION OF URANIUM ALLOYS

Investigators: L. L. Wyman and J. J. Park

Scope of Work

The initial objective of this program is the development of highly accurate constitutional diagrams of selected binary alloys of uranium. Inasmuch as the study systems are so selected as to represent related additive metals (initially U-Grp V (-Cu, -Ag, -Au), and presently the 6 platinide metals of the transition group and Re), the resulting family of diagrams provides a basis for fundamental studies of alloying relationships. These studies potentially lead to the development of a workable theory of alloying. Additionally, accurate knowledge of the binary diagrams, as well as the alloys used for these studies, provide the means for subsequent studies of reaction kinetics in these systems.

The present program status is such that the U-Pt system has been completed and the results recently published; the U-Pd and the U-Ru systems are near completion and should be published soon. The investigation of the U-Rh system is well advanced and certain data has been obtained on the U-Os, U-Ir, and U-Re systems. From the information thus far obtained, certain striking similarities in the intermetallic compound formation have been noted in alloys of high uranium on the pseudo-binary side of the usually present UM_3 compound. Obvious dissimilarities have been noted in the high platinide-metal pseudo-binary portions of the diagrams.

Contractor: New York University, New York, N. Y.

Contract: AT(30-1)-1902

Brief Title: STUDY OF THERMODYNAMIC PROPERTIES OF ZIRCONIUM-RICH ZIRCONIUM-OXYGEN ALLOYS

Investigators: K. L. Komarek

Scope of Work

A method has been developed to determine thermodynamic properties of alloys with extremely low vapor pressures, and this method has been applied to the study of titanium-, zirconium-, and hafnium-oxygen alloys. Thin specimens in contact with magnesium oxide are equilibrated with magnesium vapor from a source kept at constant temperature. The specimens are heated in a temperature gradient and their weight increase, due to oxygen pick-up, is determined by weighing. The treatment is repeated until no further weight increase is obtained. From the known free energy of the reaction between magnesium oxide, magnesium vapor, and oxygen, and the known vapor pressure of magnesium as a function of temperature, the partial molar free energy of oxygen in the alloys can be calculated.

Both the titanium-oxygen and the zirconium-oxygen system have been investigated from 800° to 1000°C between 5 and 25 at% oxygen. The partial molar free energy of oxygen in titanium increases from about -102 Kcal/g-atom O at 25 at% O to-117 Kcal/g-atom O at 5 at%O. The partial molar free energy of oxygen in zirconium in the same concentration range is about 1-2 Kcal more negative. An approximate value of -128 Kcal and -131 Kcal has been obtained for the partial molar enthalpy of oxygen in titanium and zirconium respectively.

The rate of weight increase of non-equilibrated specimens in the temperature range investigated is highest for zirconium and lowest for hafnium. The order is Zr> Ti >Hf and the ratio is approximately 10:4:1. It is thought that this method can be used to determine relative diffusion constants in similar systems.

The investigation of the titanium-, zirconium-, and hafnium-oxygen system will be completed, the data evaluated, and compared with results published in literature or obtained from statistical mechanical models. Measurements of activities and activity coefficients of magnesium in titanium-, zirconium-, and hafnium-magnesium alloys will be continued.

Contractor: New York University, New York, N. Y.

Contract: AT(30-1)-1837

Brief Title: PROPERTIES OF SODIUM-POTASSIUM ALLOYS

Investigators: B. R. Sundheim

Scope of Work

A portion of this work is devoted to the determination of the thermodynamic properties of sodium-potassium alloys as a function of composition in the range 250 to 350°C. The concentration of the two components in the gas phase above the liquid metals is determined spectrophotometrically. By comparison with the concentrations found over pure metals under the same conditions the fugacities may be obtained and thereupon the various thermodynamic properties of the liquids.

The second portion of this work concerns the behavior of solutions of alkali metals in ammine solvents at inert electrodes. Pulse methods are being used to examine the electron transfer step.

Contractor: Pennsylvania State University, University Park, Pennsylvania

Contract: AT(30-1)-2541

Brief Title: A STUDY OF HIGH TEMPERATURE PROPERTIES OF TITANIUM AND ZIRCONIUM PHOSPHIDES AND RELATED REFRACTORY MATERIALS

Investigators: Karl A. Gingerich

Scope of Work

The principal objectives of this research are to study the high-temperature properties of refractory materials with particular emphasis on the phosphides of Ti and Zr.

During the coming year methods for the preparation of pure refractory phosphides will be further developed and vapor phase reactions included. The investigation of the constitution of the binary systems will be continued by using x-ray powder analyses (both, after quenching the samples and at the temperatures of investigation) as the main tool. Systems involved will be Ti-TiP, Zr-ZrP, Nb-NbP, Ta-TaP and the phosphides of lanthanium, cerium, and thorium.

Apparatus for the measurement of phosphorus dissociation pressures will be set up and a suitable static method will be developed by investigating the titanium phosphides first. Melting points of various refractory phosphides will be measured using induction heating and their thermal expansion will be determined by high-temperature x-ray diffraction. The measurement of electrical properties at high-temperatures is anticipated.

The investigation of the influence of temperature on the ThO_2 -Eu_2O_3 system will be concluded by a series of measurements at 1900°C.

Contractor: Pennsylvania State University, University Park, Pennsylvania

Contract: AT(30-1)-2781

Brief Title: COBALT OXIDES (HIGH TEMPERATURE STABILITY RELATIONS AMONG COBALT OXIDES, AND THEIR ACTIVITIES IN SOLID SOLUTION CRYSTALS.)

Investigators: Arnulf Muan

The purpose of the present research is to contribute to the knowledge of thermodynamic properties of inorganic substances at elevated temperatures. Modern ionic approaches to the thermodynamic treatment of oxide equilibria will be tested experimentally on cobalt oxides and the solid solution series CoO-MgO and CoO-MnO.

The first step in the investigation is to delineate accurately the stability relations existing among the cobalt oxides, CoO, Co_3O_4 and Co_2O_3, including a study of the possible deviations from stoichiometry within each homogeneous phase as a function of temperature and oxygen potential. These deviations, if they exist, will be treated thermodynamically. Particular attention will be paid during this phase of the experimental work to the possible appearance of the "boundary anomaly" observed in transformations among manganese oxides.

The second step in the investigation is to study the effect of MgO additions on the non-stoichiometry of CoO, and to determine activities of CoO in CoO-MgO and CoO-MnO solid solutions in contact with metallic cobalt. The results will be treated thermodynamically and compared with similar data for NiO- and FeO- containing solid solutions.

Contractor: Pittsburgh, University of, Pittsburgh 13, Pennsylvania

Contract: AT(30-1)647

Brief Title: THERMAL AND STRUCTURAL STUDIES OF ALLOYS

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 constitutions, thermal properties and magnetic and electrical behavior of selected systems. Toward these ends work is being carried out dealing with the following topics: (1) constitution of the vanadium-hydrogen system at temperatures between 78 and 500°K, (2) heat capacity anomalies of the tantalum-hydrogen system for alloys in the vicinity of the composition Ta_2H, (3) studies of lanthanide-hydrogen systems, (4) heat capacity of $MgCd_2$, (5) x-ray line intensities for KCl-KBr at low temperatures, (6) heat capacity of intermetallic compounds having the formula AB_5, in which A represents a lanthanide element and B is iron, cobalt or nickel.

The vanadium-hydrogen system is being studied to see if a simple substitutional solid solution forms for moderate hydrogen concentrations. Ta-H alloys are being examined because in this system the interstitial hydrogens form a superlattice which is apparently destroyed in several stages as the temperature is raised. Measurements are being made to ascertain whether the destruction involves two or three stages. Thermodynamic, structural, electrical and magnetic characteristics of the lanthanide-hydrogen systems are being examined. One of the points of interest is to ascertain whether the negatively-charged hydrogen ion acquires its electron from the core electrons or from the conduction band. The work on $MgCd_2$ is part of a continuing series of studies dealing with magnesium-cadmium alloys. The study of the KCl-KBr system is for the purpose of finding whether or not the chloride and bromide ions are randomly distributed over the anion sites. The objective of the heat capacity studies dealing with AB_5 compounds is to investigate the thermal anomalies associated with certain magnetic transformations in these compounds.

Contractor: Rensselaer Polytechnic Institute, Troy, New York

Contract: AT(30-1)-2159

Brief Title: MECHANISM OF THE EFFECT OF RARE-EARTH SOLUTES ON THE ALLOTROPIC TRANSFORMATION TEMPERATURE OF ZIRCONIUM

Investigators: Arthur 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-Y, 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: RIAS, Baltimore, Maryland

Contract: AT(30-1)-2531

Brief Title: ELECTRON MICROSCOPE INVESTIGATION OF ALLOTROPIC TRANSFORMATIONS

Investigators: Henry M. Otte

Scope of Work

Allotropic transformations in a number of metals and alloys are being investigated using primarily electron transmission microscopy and selected area diffraction. It is hoped to determine, by direct observation, the mechanism of transformation in thin films and interpret the observations in terms of the dislocations involved and their movement. To cover the transformation between the three most frequently occurring structures (FCC, BCC, and hexagonal) in metals, a series of appropriate alloys will be selected. For transformations in a more complex system, alloys such as Au-Cd in the region of 50 atomic pct. will be chosen. Samples from specimens transformed by differenc amounts will be examined before and after various histories by means of heat-treatment, mechanical deformation and radiation damage. Heating, cooling and deformation of the specimen while under observation is planned.

Contractor: A. O. Smith Corporation, Milwaukee, Wisconsin

Contract:

Brief Title: EQUILIBRIUM STUDIES OF REFRACTORY METAL OXIDES

Investigators: James H. Healy

Scope of Work

This program consists of a study of the equilibria between refractory metal oxides and will entail determination of the phase equilibrium diagrams between binary oxides. Emphasis during the initial stages of the program has been placed upon the Ta-Nb-O, Ta-W-O, and Nb-W-O systems. X-ray diffraction techniques and metallography will be the primary tools utilized for equilibrium determination.

Contractor: Syracuse University, Syracuse, New York

Contract: AT(30-1)-1910

Brief Title: PHASE EQUILIBRIA: STUDIES OF SYSTEMS INVOLVING THE ALKALI AND ALKALINE EARTH METALS

Investigators: Frank A. Kanda and Aden J. King

Scope of Work

This project is concerned primarily with the investigation of the phase equilibria in systems involving alkali and alkaline earth metals. A particular system may involve members of either one or both families. After the studies of the systems involving metals containing one or two valence electrons the investigations will be extended to include metals possessing three valence electrons (e.g., aluminum and the rare earths.) as one of the components. These metals characteristically form rare-gas-type ions. One of the objectives of these studies is to observe what effect, if any, such electronic structures have on the nature of the alloy system and intermediate phases which form. The effect of the allotropic forms of calcium and strontium on alloys rich in these elements is being studied. Extensive use is being made of high temperature x-ray methods for these investigations. It became necessary to develop methods for the purification of barium and strontium in order to obtain reliable phase studies of their systems. Studies have been completed for the systems: Ca-Sr; Ca-Mg; Ca-Ba; Ba-Sr; Ba-Li and Li-Na. Work is in progress for the systems: Ba-Na; Ca-Li; Sr-Li; Sr-Na and the intermediate phases of the Mg-Sr systesm.

Contractor: Tennessee, University of, Knoxville, Tennessee

Contract: AT-(40-1)-1068

Brief Title: CALORIMETRIC MEASUREMENTS ON 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 thermodynamic properties of metal systems in the temperature range extending from room temperature to 1000°C. Related phenomena such as metastable states and non-equilibrium imperfection concentrations as revealed by energy absorption-temperature data are also being investigated. An experimental method has been developed which yields specific heat data with an accuracy better than ± 1% up to 700°C.

Specific heats and heats of transformation in several alloy systems are being investigated. These include alloys in the titanium-hydrogen system with compositions extending to the pure hydride phase, alloys in the copper-antimony system associated with the decomposition of the beta and epsilon phases, and an alloy of the Ni_4Mo composition in the Ni-Mo system.

A program of investigation of the specific heats of the solid solution phases based on copper or nickel with several solute elements is also under investigation. Measurements have been completed on Cu-Ni solid solutions and are in progress on Cu-Al, Cu-Si, Cu-Ge, Cu-As, Ni-Mo and Ni-Cr. Results indicate that the Kopp-Neumann rule applies very well for the Cu-Ni alloys. The rule applies for the systems, Cu-Al, Cu-Ga, Ni-Mo, near room temperature but an anomalous increase in the specific heat occurs at higher temperatures.

Contractor: Tufts University, Medford, Massachusetts

Contract: AT(30-1)-1410

Brief Title: FUNDAMENTAL PROPERTIES OF LIGHT METAL HYDRIDES

Investigators: Charles E. Messer

Scope of Work

The primary purpose of the contract is to obtain phase equilibrium and calorimetric data on systems of lithium hydride with structurally related compounds, and to interpret the data structurally and thermodynamically. Solid-liquid equilibrium by thermal analysis, hydrogen dissociation pressures, x-ray crystallography of novel phases, and heats of reaction are included.

In recent years, papers on systems of lithium hydride with lithium metal and with lithium fluoride have been published. Systems of lithium hydride with calcium hydride, lithium oxide, titanium hydride, and zirconium hydride also have been studied.

Currently, the thermal analysis apparatus has been reconstructed with a view to obtaining higher precision and semi-automatic operation. Systems of lithium hydride with barium hydride, strontium hydride, lanthanum hydride, and cerium hydride are currently being investigated.

A survey report on the unclassified literature on lithium hydride (NYO-9470) has been issued, combining and updating two earlier survey reports.

Systems of fluorides are of interest because of analogies with hydrides. In this work, thermal analysis of systems of lithium fluoride with the closely structurally related compounds magnesium fluoride and magnesium oxide is being undertaken. A survey of complex light metal fluorides also is in progress with a view to predicting the existence of analogous hydride complexes.

Contractor: Washington, University of

Contract: AT(45-1)-1375

Brief Title: PHASE TRANSFORMATIONS IN A EUTECTOID BINARY ALLOY SYSTEM

Investigators: Douglas H. Polonis and Raymond Taggart

Scope of Work

The project involves a continued study of the mechanisms and kinetics of transformations in binary eutectoid systems. In one part of this study an investigation is being made into the effects of alloy composition and tempering temperature on the decomposition reactions in substitutional martensitic phases. High purity alloys of titanium and copper containing 0-10 weight percent copper undergo transformation from the beta phase (b.c.c.) to alpha prime (h.c.p.) during quenching, and these alloys are at present under investigation. The tempering of alpha prime is being studied by means of x-ray diffraction, electrical resistance measurements and microscopy. The precipitation of Ti_2Cu in both equiaxed supersaturated alpha and martensite (alpha prime) will be studied in alloys containing 1.5 weight percent copper and less. This section of the program will enable the study of the effects of alpha morphology and the strain which accompanies the martensite reaction on the nucleation and growth of Ti_2Cu during decomposition.

In a further extension of the project the study of decomposition reactions in high temperature phases during quenching and aging will be initiated. This work is directed particularly toward advancing our understanding of the mechanism and kinetics of omega phase formation during quenching and subsequent aging in zirconium alloys (Zr-V, Zr-Ni).

Contractor: Yale University, New Haven, Connecticut

Contract: AT(30-1)-2723

Brief Title: THE STRUCTURE AND ASSOCIATED PROPERTIES OF IONIC SOLID SOLUTIONS

Investigators: W. D. Robertson

Scope of Work

A systematic investigation of the physical and chemical factors governing the constitution of binary, ionic solid solutions is being undertaken. As a basis for a systematic study of the factors limiting solid solubility, the saturations solubility of all alkali fluorides in lithium fluoride will be determined as a function of temperature. The investigation will then be extended to the other potassium halides, polyvalent (cation) fluorides and polyvalent (anion) oxides and sulfides.

Following a determination of equilibrium solubility, in terms of size and charge of both anion and cation, individual systems will be selected for detailed investigations with respect to; (a) the number and type of defects, (b), the structure and kinetics of precipitation, and (c), deformation and fracture phenomena.

Section I-D

Liquid Properties and Reactions

Contractor: Arkansas, University of, Fayetteville, Arkansas

Contract: AT(40-1)-2096

Brief Title: STUDY OF THE STRUCTURE OF LIQUIDS BY X-RAY DIFFRACTION

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

Scope of Work

This project involves a study of the structure of various liquids by x-ray diffraction. The scope of the research includes:

a) Study of the structure of halide complexes of the transition metals in aqueous solution. These studies are to be extended to halides other than chlorides and will include determination of the effect of temperature and of added halide ion.

b) Study of alkali metals. X-ray structural information on liquid rubidium and cesium is not currently available in the literature. These liquids, their alloys, and the alloys of other binary alkali metal systems are to be studied.

c) Study of Liquid krypton. Pending construction of low temperature apparatus the previously proposed study of liquid krypton is to be undertaken.

Contractor: Brookhaven National Laboratory, Associated Universities, Inc. Upton, Long Island, New York

Contract: AT(30-2)-Gen-16

Brief Title: ALLOY THEORY

Investigators: J. R. Weeks and D. H. Gurinsky

Scope of Work

The structure of liquid alloys is being investigated both theoretically and experimentally. One goal is a better understanding of the interactions between solid and liquid metals and the corrosion by liquid metals. Emphasis is being placed upon the thermocouple potentials generated in liquid metal corrosion, and the effects the currents so generated might have on the kinetics and mechanism of liquid metal corrosion. The steel most sensitive to selective attack has been found to be electropositive to all the others commonly tested as containers for heavy liquid metals. D.C. currents have been shown to cause Fe to migrate through liquid Bi towards the anode and Cr towards the cathode.

A statistical and quantum-mechanical approach to the theory of liquid alloys, and of metals in general, has been started. The former is based upon the theory of significant structures in liquids. Experimental data on physical properties of these alloys, and their magnetic susceptibilities will be obtained to evaluate this theory. The quantum-mechanical approach to the theory of metals is based upon introducing covalent bond theory into the molecular orbital theory of metals. It is hoped in this way to achieve one theory that explains both the band structure and the binding energies of metals.

The kinetics of reactions between solid and liquid metals are being studied with particular emphasis upon the formation of surface deposits on the solid metal and the effects of these deposits on the kinetics of dissolution of the solid metal into the liquid metal. Methods have now been perfected whereby thin, uniform deposits can be formed reproducibly; these will serve as a basis for the future kinetic studies.

Contractor: Carnegie Institute of Technology, Pittsburgh, Pennsylvania

Contract: AT930-1)-1024

Brief Title: ELECTROCHEMICAL STUDIES OF NON-AQUEOUS MELTS

Investigators: G. Derge

Scope of Work

The long range objectives of this contract have been to extend scientific knowledge of the characteristics of high temperature non-aqueous melts as typified by fusions of sulfides, oxides and salts. The study has been based on direct measurements at temperature. These are subject to physical-chemical interpretation and a variety of appropriate experimental procedures have been developed for work up to 1600°C. Emphasis has been placed on electrical conductivity and electrolysis but the information has been supplemented with data on diffusion, density, surface tension, thermoelectric power and Hall effect.

As a class, molten sulfides exhibit a wide range of electrochemical behavior and interest has centered on the Cu-S and Fe-S systems which are similar to solid semi-conductors. Sharp discontinuities in electrical conductivity occur at the stoichiometric compositions for Cu_2S and FeS. Self diffusion coefficients of iron and copper give no indication of the formation of large complexes. Hall effect measurements and calculations show that both electrons and positive holes may act as current carriers in these systems. The work will be completed by pertinent information on nickel and cobalt sulfide systems.

The molten sulfides would be expected to have a large Seebeck potential which has been confirmed in a number of cases. A systematic study of this problem has been made on melts of thallium with V and VI group elements; the latter show a high Seebeck potential.

Hall effect data show that the conducting species and mechanism in molten metallic and sulfide systems can be evaluated and the wok will be extended to include variation with composition for correlation with conductivity data.

Self diffusion data for aluminum in molten silicate slags has shown that the amphoteric behavior of this element can be correlated with the slag structure. Other studies of density in iron silicate show that in the highly basic compositions an oxide network is dominant over the silicate network associated with acid slags. Conductivity in the $CaO-Al_2O_3$ system is sensitive to the addition of calcium carbide and this will also be used as a tool to gain further understanding of basic slag structure.

Contractor: Carnegie Institute of Technology, Pittsburgh, Pennsylvania

Contract: AT(30-1)-2360

Brief Title: THERMAL CONDUCTIVITIES OF INORGANIC MELTS

Investigators: William O. Philbrook

Scope of Work

An apparatus has been designed for determining the thermal conductivity of inorganic melts, such as sulfides, silicates and halides, in the terperature range from 800° to 1200°C, and electrical instrumentation has been procured. The apparatus will be a thermally guarded, concentric cylinder, steady-state apparatus for absolute determination of thermal conductivities. Graphite will be used for the initial apparatus, to be used for molten sulfides and other salts compatible with graphite.

The tungsten-graphite thermocouple, using a film of molten metal (e.g.aluminum) as the hot junction, has been investigated because it offers design advantages, but tests of homogeneity and reproducibility have not yet been completed because of experimental difficulties. An alternate thermocouple pair is available.

Results will be useful for correlation with other transport properties of these melts to aid in elucidating their structure, for evaluating the figure of merit of certain melts that may be useful in thermoelectric devices, and for engineering purposes in metallurgical and ceramic processes.

Contractor: Delaware, University of, Newark, Delaware

Contract: AT(30-1)-2722

Brief Title: STATISTICAL THERMODYNAMICS OF METALLIC SOLUTIONS

Investigators: L. P. Skolnick

Scope of Work

Prior work indicates that the models used by the chemists, while satisfactory for many non-electrolytic or non-electronic solutions, are inadequate for understanding the thermodynamic behavior of metallic solutions. It is proposed to use the methods of statistical thermodynamics to derive equations analogous to those presently used for ordinary chemical solutions, but to include electron-ion interactions in the model. The models are to be critically examined in terms of electronic behavior and the equations checked for consistency with thermodynamic data.

A computer program will be used for a regression analysis of experimental data in terms of derived equations. The thermodynamic data will be obtained from other investigators and from a modest experimental program for some systems as suggested by the theoretical development.

Work is to be initiated for the study of the compositional dependence of electronic behavior in order to test the models used and to suggest other approaches. This portion of the program is to be a common effort of metallurgists and physicists. Plans are to use measurements of the work function as an indication of the Fermi level on a macroscale; and to use nuclear magnetic resonance to study local electronic environments.

Contractor: Massachusetts Institute of Technology, Cambridge, Massachusetts

Contract: AT(30-1)-1888

Brief Title: ACTIVITIES IN LIQUID AND SOLID METAL SYSTEMS

Investigators: John F. Elliott

Scope of Work

The research being carried out under this project is directed towards obtaining more complete information on the thermodynamic properties of metallic solutions. Also, some of the work is directed to a better understanding of the reasons for the behavior of metallic solutions. The project is a vital portion of a broader program on high-temperature solution calorimetry, solubility of gases in metals, and the thermodynamic properties of metallic solutions.

The thermodynamic studies is process this year are directed to obtaining a better general model than Henry's Law provides for estimating the activity coefficient of a dilute component in an alloy system having a large miscibility gap. Experimental results from the Al-Pb-Bi and Mn-Pb-Bi systems are being used to guide the selection of a model. Data on the solubility of gases in liquid metals (from related experimental work) are being incorporated into the theoretical study.

A search is being made for a reversible emf cell having a fused electrolyte that can be used above 1200°C. If successful, this will permit work on a number of additional metal systems.

The study of the factors influencing the chemical potential of the pure manganese which precipitates on cooling from a lead-manganese solution is now being completed. It is hoped that this problem of precipitation of a solid metallic phase from a liquid metallic phase will be continued next year.

Contractor: Massachusetts Institute of Technology, Cambridge, Mass.

Contract: AT(30-1)--1985

Brief Title: KINETICS OF REACTIONS BETWEEN LIQUID ALLOYS AND MOLTEN SALTS

Investigators: Thomas B. King

Scope of Work

The work under this contract is intended to elucidate the mechanism of reactions between a metallic alloy and an ionic liquid, such as a fused salt, which are in contact along a phase boundary. In such systems displacement reactions, for example, consist of transport steps, by diffusion and convection within the two liquids, and reaction at the phase boundary.

It can be shown that if overall transport control prevails and the transport of only one species is rate-controlling, the rate constant is proportional to the square root of the diffusion coefficient of that species. Rate studies and measurements of diffusion coefficients to establish this have been made on the general type of system,

$$M_1 \text{ (in alloy)} + M_2 + \text{(in halide)} = M_1 + \text{(in halide)} + M_2 \text{ (in alloy)}$$

Rate control by transport in both alloy and salt have been demonstrated.

In reactions involving gas evolution or reduction of a complex ion, over-all rate control by the phase boundary reaction is possible. Rate measurements are being made on systems such as,

$$SiO_2 \text{ (in silicate)} + \frac{4}{3} Al \text{ (in copper)} = Si \text{ (in copper} + \frac{2}{3} Al_2O_3 \text{ (in silicate)}$$

under varying convection conditions.

Electrolytic polarization techniques are also being actively pursued for study of both types of reaction with major emphasis on activation control.

Diffusion coefficients are also being measured to aid in the interpretation of direct rate measurements.

Examples of mixed activation and transport control will also be examined under varying convection conditions. Tracer measurements will be necessary for some systems to establish with certainty that activation control is operative.

Contractor: Michigan, University of, Ann Arbor, Michigan

Contract: AT(11-1)-771

Brief Title: TRANSPORT PROPERTIES IN LIQUID METALS

Investigators: Edward E. Hucke

Scope of Work

The work on "Transport Properties in Liquid Metals" is aimed at better understanding of the structure of liquid alloys. Specifically, this program utilizes the theory of irreversible thermodynamics to provide a framework for correlation between measured electric mobility data and known thermodynamic functions in liquid Bi-Sn alloys. Electric mobilities are measured with a resistivity techniques previously developed. From these data the effective charges of the metal atoms can be deduced. The validity of the irreversible theory is checked by measurements of the electric diffusion potential.

Contractor: Michigan, University of, Ann Arbor, Michigan

Contract: AT(11-1)-979

Brief 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 the following activities:

1. A summary of currently available data on liquid ternary solutions will be tabulated in the form of interaction parameters.

2. A study of the effect of third element additions on the activity of cadmium in liquid tin will be initiated using the electromotive force technique. Consideration will also be given other ternary systems for which the properties of two or more of the associated binary systems are known.

3. A study of the solubility of nitrogen in liquid nickel and cobalt alloys will be made using the Sieverts' method. The solute interactions between dissolved nitrogen and a third element will be compared for the solvents, iron, cobalt, and nickel.

Contractor: Michigan, University of, Ann Arbor, Michigan

Contract: AT(11-1)-543

Brief Title: INVESTIGATION OF THERMODYNAMIC ACTIVITIES AND SOLUBILITY RELATIONSHIPS IN BISMUTH SYSTEMS

Investigators: David V. Ragone, Edward E. Hucke and Richard E. Balzhiser

Scope of Work:

The first part of the investigation is concerned with the determination of thermodynamic activities in metallic systems using a vapor pressure method. These vapor pressures are determined by an optical absorption technique. This technique allows separate determination of pressures of monatomic and diatomic species in the vapor. Current efforts are being made on the U-Bi, Au-Cd, and Bi-Te systems. The effect of pressure broadening on absorption lines is being investigated.

The second portionof the investigation is concerned with interactions between uranium and other solutes in bismuth solutions. This has been studied by measuring the solubility of uranium as a function of Pd and Cu additions. The decomposition of uranium dicarbide in bismuth was also studied as a function of Pd and Cu additions. Future work will involve elements near Pd and Cu in the periodic table.

Contractor: Minnesota, University of, Minneapolis, Minnesota

Contract: AT(11-1)-841

Brief Title: DIFFUSION STUDIES IN LIQUID METALS

Investigators: Richard A. Swalin

Scope of Work

The purpose of the research program is to obtain experimental information which will be useful in elucidating the mechanism of atom movements in the liquid state. Recently theories of liquid state diffusion have been proposed by Cohen and Turnbull and by Swalin. These predict different types of temperature dependence of the diffusion coefficient. We propose to investigate the self diffusion coefficient of tin-113 in tin over a wide temperature interval in order to look for effects proposed by these theories.

Studies of the diffusion constant of lead in tin will also be performed in order to complete our investigation of solute diffusion coefficient versus relative partial molal enthalpy.

A study of solute diffusion in liquid silver is being initiated. Theoretically speaking, silver base systems are advantageous since more is known about the electronic states of these systems than most others. In particular diffusion of silver, cadmium, indium, tin and antimony in silver will be investigated.

Contractor: Oklahoma, University of, Norman, Oklahoma

Contract: AT-(40-1)-2409

Brief Title: DIFFUSION PHENOMENA IN LIQUID METALS

Investigators: W. R. Upthegrove

Scope of Work

This research is a study of diffusion phenomena in liquid metal systems to obtain an improved understanding of the effects of system variables upon these phenomena and of the diffusion mechanisms involved.

The investigation of diffusion in very dilute solutions, specifically the iron-mercury system, is continuing. The influence upon diffusion by metallic additive agents which are utilized to inhibit mass transfer in this system is being evaluated. An analysis of the published data for diffusion-rate controlled mass transfer in this system will be completed.

Self-diffusion and inter-diffusion coefficients for the lead-cadmium system using the capillary-reservoir method are being determined. An evaluation of these data in terms of Darken's equation relating these coefficients and thermodynamic parameters is planned.

The Research will be extended to include a basic study correlating viscosity and diffusion for the Group II-B liquid metals. This study will include viscosity measurements for zinc-mercury and cadmium-mercury amalgams as a function of temperature and composition. Diffusion coefficients will be determined at compositions such that the amalgams are isoviscous solutions, i.e., solutions exhibiting coincident viscosity-temperature curves.

Contractor: Purdue University, Lafayette, Indiana

Contract: AT(11-1)-359

Brief Title: DIFFUSION IN LIQUID ALLOYS

Investigators: Richard E. Grace

Scope of Work

The long range purposes of this investigation are to determine rates and mechanisms of diffusion in liquid alloys and corrosion of solids in liquid alloys. At the present time the following work is in progress:

a. $Zinc^{65}$ is being used as a tracer to measure self diffusion of zinc in homogeneous lead-zinc alloys by the capillary-reservoir method. Compositions up to two weight percent zinc and temperatures in the range 350 to 600°C are being investigated.

b. The rate of solution of rotating aluminum cylinders in liquid bismuth is being measured. Solubility data for the liquidus line between 300 and 600°C have been obtained for the aluminum-bismuth system, and preliminary results of dissolution experiments indicate that the process is controlled by diffusion in the liquid phase.

c. The rate of solution of copper in liquid lead in an isothermal loop is being investigated. Copper test sections are placed in one leg of a stainless steel loop in which liquid lead is pumped. The temperature interval being studied is from 400 to 600°C.

Contractor: Stanford University, Stanford, California

Contract: AT(04-3)-283

Brief Title: THERMODYNAMIC AND TRANSPORT PROPERTIES OF LIQUID METAL SOLUTIONS

Investigators: David A. Stevenson

Scope of Work

Research is currently in progress on the thermodynamic and transport properties in liquid metal solutions.

The thermodynamic studies are concerned with phase distribution between solid and liquid phases, primarily in binary systems. In many instances, unreliable and erroneous data are available. An accurate knowledge of phase distribution allows calculation of the differential heat of solution and the excess partial molar entropy. The eventual aim of this study is to correlate these thermodynamic quantities with basic physical parameters of the solvent and solute similar to corresponding analyses in molecular solutions. The bismuth-chromium system is currently under investigation.

The transport properties currently being studied are the isothermal transport across solid-liquid phase boundaries and solid state diffusion. Studies of the first property seek to distinguish the rate limiting mechanism involved under differing conditions. The essential variables involved are: the solid-liquid system; temperature; grain size and orientation; and the hydrodynamic conditions relating to the relative flow of solid and liquid. The solid state diffusion studies are being made to show what changes occur in the solid composition during mass transport across solid-liquid phase boundaries. The system zinc-mercury is currently under investigation using radioactive isotopes.

Contractor: Syracuse University, Syracuse, New York

Contract:

Brief Title: INVESTIGATION OF SPECIFIC VOLUMES OF LIQUID METALS AND ALLOYS

Investigators: F. A. Kanda and D. V. Keller, Jr.

Scope of Work

At the present time, the data on the specific volumes of liquid alloy systems are not complete enough to warrant an extended investigation of the relationships between specific volume and nature of metals in the liquid state. Precise data of this nature are necessary for the determination of the values of viscosity, thermodynamic relationships and other liquid properties. The purpose of the proposed research is to: (1) determine the ultimate accuracy and reliability of the "densitometer" techniques, and (2) then proceed to investigate a series of liquid metal alloys at various temperatures. The initial investigations will include the critical region of an immiscible system. These data should ultimately produce logical generalizations regarding attractive forces between metal atoms in the liquid state.

Contractor: Union Carbide Nuclear Company, Oak Ridge National Laboratory, Oak Ridge, Tennessee

Contract: W-7405-eng-26

Brief Title: SPECTROSCOPY OF IONIC MEDIA

Investigators: G. P. Smith, C. R. Boston, and J. J. McBride

Scope of Work

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 concerned with charge-transfer spectra of several types and with spectra of solutions of metals in molten salts. Two 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 post-transition metals.

Contractor: Yale University, New Haven, Connecticut

Contract: AT(30-1)-2029

Brief Title: STUDY OF METALLIC LIQUIDS

Investigators: R. B. Gordon

Scope of Work

Scope I, Ultrasonic Measurements

Measurements of the compressibilities of liquid mercury-thallium alloys have been made as a function of temperature and composition. The results, in contrast to earlier x-ray observations, give no indication of the occurrence of non-random, liquid structures at the composition 28 atomic percent thallium, but do reveal a very marked decrease in the compressibilities of the dilute alloys. In further investigation of this effect dilute alloys of mercury with Pb, Sn, In, Zn, Cd, and Bi have been investigated; all show a very large decrease in compressibility. The explanation of this effect in terms of the type of bonding in liquid mercury now is being considered. Compressibility data are being obtained for the sodium-potassium system.

Scope II, Galvanomagnetic Measurements

A study of the variation of the Hall coefficient with the degree of order and antiphase domain size in the alloy Cu_3Au has been completed. The alloy Au_3Cu is also being investigated and apparatus is being constructed for Hall coefficient measurements in liquid alloys.

Contractor: Yale University, New Haven, Connecticut

Contract: AT(30-1)2560

Brief Title: X-RAY STUDY OF LIQUID METALS

Investigators: C. N. J. Wagner

Scope of Work

Increased interest in the physical properties of dilute alloys of mercury has lead to the x-ray study of their structures. The diffracted intensity from pure mercury has been measured with two different experimental methods, and the results agree very well with the latest literature values. Dilute alloys of Hg with Pb, Sn, Bi, Tl, In, Zn, and Cd will be studied at room temperature.

Binary alloys of Ag-Sn and In-Sn will be studied at elevated temperatures. A high-temperature and high vacuum x-ray diffractometer attachment was purchased and altered to meet the requirements for the x-ray study of high melting liquids. The reason for the study of the Ag-Sn system is that many other physical properties like viscosity and electrical resistivity are known, whereas in the case of In-Sn it is hoped that the compressibility could be evaluated from measurements of the velocity of sound in the liquid.

Section I-E

Corrosion, Oxidation, and Surface Phenomena

Contractor: Argonne National Laboratory, Lemont, Illinois

Contract: W31-109-eng-38

Brief Title: BASIC CORROSION RESEARCH

Investigators: F. E. DeBoer, J. E. Draley, R. K. Hart, R. D. Misch, S. Mori, W. E. Ruther

Scope of Work

The objective of this research progrm of this group is to isolate and measure the factors which control the corrosion of metals in water and steam over a wide range of temperatures. The metals of interest, primarily aluminum, zirconium, uranium and their alloys, owe their corrosion resistance to the presence of films of oxide or hydrated oxide. Much of the investigation is thus concentrated on film properties and structure and their relationship to alloy composition. Electrical properties are of particular interest and measurements are being made of polarization potentials in water and of the e.m.f. of the growing scale in dry oxygen. Precise determination of the corrosion kinetics is being made for prolonged exposure of aluminum in water. Additions to the water are of minor interest, but have been studied in the past. A more detailed description of the major programs is given below:

Scope I Aluminum in Water and Steam

At temperatures from 50° to 100°C the pH change at the surface at 1100 aluminum and the fraction of corrosion product which dissolves have been determined during the period of rapid film growth. Dissolved corrosion product causes an increase in corrosion rate and this fact is reflected in the influence of flow rate and on the position of one specimen relative to another. The reason for this influence is still unknown. After several days the corrosion rate becomes low with no transition appearing even after one to two years. Attempts are being made to account for the different features of the corrosion curve based on the observed topographical changes.

At temperature of 290° (water) to 540°C (steam) the corrosion rate is very sensitive to various alloy additions. Alloys containing nickel, iron and titanium have excellent corrosion resistance which is adversely affected by as little as 110 ppm Si at 305°C. At higher and lower temperatures the effect of such low Si contents is much less critical. A number of obvious possibilities have been eliminated and the mechanical strength of the film is now considered as an important variable. Specimens are being studied in the form of spheres to see if the anomalous rate at 305°C is still observed. The effect of incorporation of silica from the water is also being studied.

In steam at 540°C, 600 psi, the destructive attack has been identified with hydrogen penetration which produces gas voids containing H_2 and steam. The corrosion product on the walls of these holes is a nonprotective form, identified by sectioning and using electron diffraction.

Scope II Zirconium in Water and Steam

Alloying elements, either singly or in combination, are believed to have at least four principal effects on the oxide layer. These effects are: structural (e.g., favoring cubic instead of monoclinic ZrO_2 at the temperature and pressure of the corrosion test), electrical conductivity of the scale (either of the ZrO_2 or because of second phases), ability to catalyze H atom combination, and mechanical strength of the oxide.

A study on a large number of binary alloys showed that optimum resistance in 540°C steam occurred for those alloys which followed the cubic rate law in 700°C, 200 mm HgO_2 and also had conducting films. The better alloys contained Co, Fe, Mo, Pt and U.

Another approach based on alloying is to use two additives, e.g., Sc^{3+} and Nb^{5+} which have an average valence of +4 and thus should not have a large effect on the defect structure of ZrO_2. A series of zirconium alloys containing 0.05 a/o A and 0.05 a/o B where A and B are two different elements is being investigated in 540°C steam. One of the best of these alloys is 0.05 a/o Pt, 0.05 a/o Ta. Some of these alloys have been oxidized in O_2 at 700°C for comparison with the steam results. E.m.f. measurements will be made in steam to determine whether film conductivity is a general feature of the more resistant alloys. This property is believed to be important in preventing hydrogen damage.

Scope III Application of Electron Microscopy and Electron Diffraction

Most of this work has used direct examination of alloy foils, evaporated films, or corrosion products (both sectioned and nonsectioned). Foils of aluminum and zirconium alloys have been examined after thinning by electropolishing or chemical polishing. The size, shape and composition of second phase particles in corrosion-resistant aluminum alloys have been identified and the effect of heat treatments have been observed. Examination of zirconium-titanium alloys did not show any metallographic changes to which the increased corrosion rate could be ascribed.

The topography of corrosion products is being examined by using 1/8" dia. discs with a hole 0.001" in the center. By viewing the edge of this surface after corrosion the growth of oxide whiskers and other formations has been observed on aluminum and zirconium alloys and on pure iron. The influence of oxygen on the corrosion rate of iron can be related to changes in the oxide surface.

Evaporated films enable a study of diffusion and precipitation in alloys of special interest. At present, the systems Al-Ni and Al-Ni-Si are being studied. The procedure involves depositing aluminum or aluminum-8% silicon alloy onto rock salt at 450°C. A nickel deposit is then deposited on top of this film. The bimetallic system is then heated at different times and temperatures and compositional changes are observed by electron diffraction. A nickel-rich compound forms first indicating the more rapid diffusion of aluminum. Silicon produces several changes which are still being investigated.

Scope IV Polarization Potentials

After surveying a number of pure metals the current program is devoted to a detailed examination of aluminum. The usual generalizations such as the Tafel relationship have only limited applicability in pure water because surface films are the controlling factor in electrolysis. The examination of films *in situ* by means of polarization curves has the advantage of not requiring any assumption concerning surface changes as would be necessary if the specimens were removed and examined in air.

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

Contract: W-7405-eng-48

Brief Title: HIGH TEMPERATURE REACTIONS

Investigators: A. W. Searcy

Scope of Work

The principal objectives of the current programs are to elucidate the equilibria 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. The ultimate aim is to acquire sufficient knowledge to predict high temperature reaction rates from knowledge of surface conditions and equilibrium data for reactants and products.

Theoretical development and analysis of models for predicting shapes and stabilities of gas molecules of possible high temperature importance is also undertaken.

Contractor: Cornell University, Ithaca, New York

Contract: AT(30-1)-1994

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

Investigators: C. W. Spencer

Scope of Work

This investigation is concerned with the penetration of liquid metals into the grain boundaries of solid metals. The effects of temperature, liquid composition, plastic deformation, and relative crystallographic orientation of neighboring crystals at the grain boundary are being explored.

At this time the program is primarily concerned with penetration of bismuth-nickel liquids into grain boundaries in oriented nickel bi-crystals. The process of grain growth in the presence of thin intercrystalline liquid films is also under investigation.

Contractor: Georgia Institute of Technology, Atlanta, Georgia

Contract: AT-(40-1)-2755

Brief Title: SURFACE PROPERTIES OF MAGNETIC MATERIALS

Investigators: Edwin J. Scheibner

Scope of Work

The purpose of the research under this contract is to investigate the surface properties of magnetic materials. The investigation consists of three phases: (1) studies of high purity films of metals and alloys; (2) the determination of the Curie temperatures in thin films; and (3) studies of the oxidation of thin films and single crystals in the vicinity of the Curie point.

The initial effort will be devoted to the studies of thin films of metals and alloys, namely, nickel, nickel-copper, and nickel-iron. Methods will be developed for the preparation of such films under carefully controlled conditions at vacua of the order of 10^{-8} Torr or less. In addition, their structure, crystalline nature, composition, thickness and impurity content will be examined. The determination of the Curie temperatures in thin films is related to the third phase where the oxidation of thin films and single crystals will be studies in the vicinity of the curie point. Measurements will be made of the magnetization and resistance as a function of temperature for films of different thicknesses and compositions. The oxidation studies will be directed mainly towards observing the growth of oxide nuclei by optical microscopy, electron diffraction, and electron microscopy. Methods for forming high-resolution replicas of the oxidized films or surfaces will be developed.

Contractor: University of Missouri School of Mines and Metallurgy, Rolla, Missouri

Contract: AT(11-1)-73, Proj. No. 5

Brief Title: CORROSION OF NUCLEAR AND OTHER METALS

Investigators: M. E. Straumanis and W. J. James

Scope of Work

1. The work is a continuation of unclassified research on corrosion of metals and includes:

(a) A study of the mechanism of dissolution of Be and of ZrN_x TiN_x, and HfO_x solid solutions in hydrofluric acid and in mixtures of hydrofluoric and hydrochloric acid. (The mechanism shall be explored using acids containing various additions and by measuring the activation energies, corrosion potentials and difference effects. The formation and composition of surface films which are growing during the dissolution experiments shall also be explored.)

(b) A study of the mechanism of dissolution of sheet hafnium in $HF-HNO_3$ mixtures as far as is possible by the means mentioned above.

(c) A difference effect study of Mg dissolving in HF and other acids and determination of valency of ions of Mg going into solution.

2. The high temperature attack by Cl_2 and HCl of Ti and Zr metals, oxides, and nitrides will be studied.

Contractor: Pennsylvania State University, University Park, Pennsylvania

Contract: AT(30-1)-1710

Brief Title: RESEARCH ON GRAPHITE

Investigators: Philip L. Walker, Jr. and Howard B. Palmer

Scope of Work

The study of the formation, properties, and reactions of pyrolytic carbon constitutes the primary goal of this program. This program is divided into two phases: (1) measurements of the kinetics of deposition of carbon films by thermal decomposition of pure gaseous compounds, plus study of the physical properties of the films and their chemical reactivities; and (2) studies of the chemical mechanisms involved in the breakdown of hydrocarbons to form carbon. In the first phase, carbon suboxide, C_3O_2, is decomposed in a flow system, yielding microcrystalline, graphitic film carbon under conditions of low concentration in a helium carrier gas at temperatures of the order of 700°C. Deposition kinetics are controlled by chemical bond-breaking reactions under these conditions. In the second phase, details of secondary processes in benzene pyrolysis are being explored. At present, a flow system study of acetylene decomposition is being refined, following the work of Slysh and Kinney on benzene, acetylene, and diacetylene.

The study of the kinetics and mechanism of reaction of carbon with oxidizing gases also is continuing. This study is divided into five phases: (1) the mechanism by which impurities catalyze the reaction of graphite with oxidizing gases; (2) the effect of impurity additions on the solid state properties of graphite (electrical conductivity, magnetic susceptibility, and thermoelectric power); (3) determination of the individual rate constants in the spectroscopic graphite-carbon dioxide reaction as a function of temperature and burn-off; (4) the effect of temperature and radiation damage on the diffusion of gases through nuclear graphites; and (5) the effect of metal substrate on the mode of growth of evaporated carbon films and their reactivity to oxidizing gases.

Contractor: Purdue University, Lafayette, Indiana

Contract: AT(11-1)-776

Brief Title: THE EFFECT OF OXYGEN PRESSURE ON THE OXIDATION OF CHROMIUM

Investigators: Richard E. Grace

Scope of Work

The general purpose of this research is to study the rates and mechanisms of high temperature oxidation processes. The current projects are as follows:

a. Work on the oxidation of chromium in damp hydrogen. The oxidation rate is to be studied at dew points from 0 to -50°C and at temperatures from 600 to 800°C. Fundamental information on the defect structure of Cr_2O_3 and the rate of growth of Cr_2O_3 on chromium will be gained.

b. Recently initiated work on the effect of chromium on the oxidation of aluminum will be continued. Oxidation of a series of dilute aluminum-chromium alloys in oxygen gas at 1 atm at temperatures from 500 to 600°C is expected to yield information on the ternary system, Al-Cr-O. In addition, diffusion paths during the oxidation process may be followed by metallographic and diffraction techniques.

Contractor: Rensselaer Polytechnic Institute, Troy, New York

Contract: AT(30-1)-2714

Brief Title: THE ELECTROCHEMICAL AND CORROSION CHARACTERISTICS OF RARE EARTH AND YTTRIUM METALS

Investigators: Norbert Greene

Scope of Work

This program consists of an extensive study of the corrosion and electrochemical characteristics of rare earth metals. Specific phases of the program include a study of the electrode kinetic behavior of these metals. Cathode reduction studies, including measurement of hydrogen overvoltage, and anodic dissolution studies also will be performed. The corrosion resistance of the rare earth metals in acids, bases, and salts, as well as the effect of temperature, oxidizers, and other variables will be determined. The corrosion behavior will be correlated with electrochemical behavior.

Contractor: Temple University, Philadelphia, Pennsylvania

Contract: AT(30-1)2775

Brief Title: A SOLID STATE STUDY OF ZIRCONIUM AND NIOBIUM OXIDES

Investigators: Robert E. Salomon

Scope of Work

Photovoltaic studies will be made with electrodes prepared by anodizing zirconium and niobium specimens. The experiments will be performed utilizing evaporated metal layers, high purity polycrystalline samples and specific crystal faces of single crystals of niobium.

It is believed that this work will facilitate an elucidation of the band structure of the oxide and the nature of the metal-oxide interface. These findings will in turn complement corrosion and electrochemical-kinetic studies previously made.

The films will be grown under carefully controlled conditions. The temperature growth rate and electrolyte will be kept constant so that a comparison of results will be feasible. The films will be coated with an evaporated metal layer that is thin enough to transmit the effective wavelength efficiently and still thick enough to provide good electrical contact. The coated electrodes will be mounted in an air-tight chamber containing a quartz window for illumination purposes. Photovoltage and photocurrent response times will be studied as functions of the wavelength, the film thickness, the temperature and the physical state of the underlying base metal. Photovoltage decay curves will be studied under similar conditions.

An attempt to measure the thermoelectric power of these various systems also will be made.

Contractor: Toledo, University, Toledo, Ohio

Contract: AT(11-1) - 1000

Brief Title: OXIDATION OF ZIRCONIUM-NIOBIUM ALLOYS; 300-500° C

Investigators: Otto Zmeskal and K. H. Lin

Scope of Work

This research is aimed at (I) the determination of the kinetics of oxidation of zirconium-niobium alloys in the temperature range, 300-500° C, over the time interval of 0 to 100 hours, and (II) at the clarification of the mechanism of oxidation using all structure measurement techniques available to us. The first part of the study will be carried out gravimetrically, using a quartz helix balance. In order to compare results with those achieved by a volumetric study (O. Zmeskal and M. L. Brey, Trans. ASM, 1960) the first runs will be conducted at 600° C. The progress of film formation will be followed metallographically and with the aid of x-ray diffraction measurements.

It is expected that the major part of this program will be devoted to the study of the thin adherent films contrasted to the thick scales that result from high temperature oxidation. Additional structure studies will be conducted by petrographic examination and ultra-violet spectrophotometry. It is also hoped that electron microscope examination of the films will yield valuable information.

Contractor: Union Carbide Nuclear Company, Oak Ridge National Laboratory, Oak Ridge, Tennessee

Contract: W-7405-eng-26

Brief Title: CHEMICAL REACTIVITY OF METAL SURFACES

Investigators: U. Bertocci, L. D. Hulett, L. H. Jenkins, T. R. Wilson, and F. W. Young

Scope of Work:

The kinetics of the electrochemical dissolution of copper crystals in deaerated $CuSO_4$ solutions is being investigated using a galvanostatic technique. Conditions have been defined for the dissolution via a dislocation mechanism; this dissolution leaves pits at dislocation-surface intersections. Other conditions of potential and current cause the surface to be faceted by the dissolution, and apparently dislocations are not involved in this mechanism. The kinetics of the dissolution of copper crystals in aqueous solutions is also being studied using conductivity and differential refractive index techniques. These experiments are designed to elucidate the role of dislocations and of crystal plane in the chemical reactivity of metal surfaces. Several etch solutions have been found which will satisfactorily form pits at dislocations on the close-packed faces of pure copper. These solutions are being used to investigate the motion of dislocations under applied stress in both annealed crystals and crystals hardened by neutron irradiation.

Contractor: Union Carbide Nuclear Company, Oak Ridge National Laboratory
Oak Ridge, Tennessee

Contract: W-7405-eng-26

Brief Title: METAL SURFACE STUDIES

Investigators: J. V. Cathcart, R. E. Pawel, and G. F. Petersen

Scope of Work

The purpose of the research is the investigation of the role of strain in oxide films in the mechanism of oxidation of metals, especially in so far as strain is a factor in determining the degree of protectiveness of oxide 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. In addition, 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 (100) crystallographic planes where both oxide and metal possess a high degree of rotational symmetry.

Contractor: Virginia Institute for Scientific Research
Richmond, Virginia

Contract: AT-(40-1)-2502

Brief Title: CORROSION OF METALS IN BOILING ACIDS

Investigators: Henry Leidheiser, Jr.

Scope of Work

(1) The platinum metals vary in their relative effectiveness in accelerating the corrosion of less noble metals in boiling acids when in electrical contact with the less noble metal. In the case of tin in boiling 2M HCl, it has been shown that dissolved tin ions vary in their ability to inactivate platinum, palladium, rhodium, and iridium as a hydrogen electrode. Additional potential studies will be made in an effort to attach quantitative values to equilibria on the palladium surface. Specificially, the decay of the potential of a palladium electrode will be followed as a function of time of coupling to a tin electrode and as a function of concentration of dissolved tin in the boiling acid.

(2) An interpretation of the corrosion of two-component solid solution alloys has been made on the base of (a) the corrosion rates of the pure components in the same medium and (b) the concentration in the surface of atoms having all like nearest neighbors. Corrosion measurements will be made on copper-gold, copper-palladium, and copper-nickel alloys in order in order to obtain additional experimental data to test the hypothesis.

Contractor: Yale University, New Haven, Connecticut

Contract: AT(30-1)-2495

Brief Title: CONTRIBUTIONS TO THE UNDERSTANDING OF "HIGH TEMPERATURE OXIDATION OF METALS"

Investigators: J. Bruce Wagner, Jr.

Scope of Work

Present studies are divided into two areas. These are (1) The Role of a Displacement Reaction in the Oxidation of an Alloy and (2) Variables Affecting the Transition from an Interface-controlled to a Diffusion-controlled Reaction.

In the case of (1), oxidation studies are carried out on homogeneous binary alloys whose constituents differ markedly in their affinity for oxygen. An intermediate isothermal anneal in an inert gas is used to demonstrate the changes in structure and composition of the oxides formed which affect the rate of the reaction.

In the case of (2), systems are chosen which may be analyzed in terms of a steady-state approximation involving the implicit assumption that the rate of entropy production is small. Iron, nickel and cobalt at temperatures of 900 to 1200°C are being reacted in well-defined ratios of CO/CO_2. The reactions obey linear kinetics until a critical thickness is obtained where the reactions obey parabolic kinetics. Experimental results are being used to confirm predicted behavior whereby the dissociation of CO_2 as the rate-determining step is superseded by the bulk diffusion step.

Section I-F

Properties of Metals and Ceramics

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

Contract: W-7405-eng-82

Brief Title: PHYSICAL PROPERTIES OF RARE-EARTH METALS

Investigators: R. G. Barnes, S. Legvold, D. T. Peterson, J. F. Smith, and F. H. Spedding

Scope of Work

The vapor pressures of the rare earths have been found to be one of the physical properties of these metals that exhibit the greatest difference from one element to the next. The vapor pressures of lanthanum, neodymium, europium, dysprosium, thulium, scandium and holmium have been measured as a function of temperature.

In several studies of ytterbium, anomalous values of some physical properties have been observed. The most unusual behavior is the tremendous increase in electrical resistivity as pressure is increased, as observed by Bridgman. Presently the magnetic susceptibility of ytterbium is being measured in an effort to determine the number and origin of the conduction electrons.

Single crystals of gadolinium have been grown by the strain anneal technique. The magnetic and electrical properties of these single crystals are being determined.

The cohesive energies of most of the rare-earth metals have been determined by our mass spectrometer method. Terbium studies and lutecium studies have recently been completed.

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

Contract: W-7405-eng-82

Brief Title: HIGH TEMPERATURE PROPERTIES OF MATERIALS

Investigators: O. N. Carlson, A. H. Daane, D. T. Peterson, and D. R. Wilder

Scope of Work

The first step in evaluating the possibility of a material for a high temperature application is to measure the properties of the material in the temperature range of interest. These data serve as a basis for theoretical and engineering developments.

Thermal expansion and x-ray reflection intensities for single crystals of copper and zinc have been determined from x-ray diffraction data taken in the temperature range from room temperature to near the melting points of the crystals. Modifications in the high temperature x-ray camera are being made so that measurements can be extended to the more refractory metals such as tantalum. These data will be helpful in understanding the temperature dependence of the thermal expansion, electrical resistivity and other properties of metals and alloys.

Resistivity measurements on gadolinium, dysprosium and some other rare-earth metals indicate the presence of high temperature forms of these metals that have not been characterized. It has been found that small additions of magnesium to yttrium make it possible to retain the high temperature form of the metal at room temperature by quenching.

The principal objective of our research on the sintering of ceramic materials is to develop a better understanding of the mechanism of the process. Materials under study include UO_2 and Y_2O_3. The emissivity of several refractory oxides are being measured in the temperature region 1500 to 2200°C using an arc-image furnace.

Contractor: Argonne National Laboratory, Argonne, Illinois

Contract: W-31-109-eng-38

Brief Title: THE PHYSICAL AND CHEMICAL PROPERTIES OF GRAPHITE

Investigators: G. R. Hennig, G. Montet, M. Kanter and M. Dzurus

Scope of Work:

The objective of this work is to increase the basic understanding of the solid state physics and chemistry of crystalline carbon, especially of graphite. Essentially all of the research deals with single crystals of natural origin since these are the best materials available to date. Attention is focused on two major areas, the defect structure of graphite crystals and their chemical reactivity.

Both point defects and extended defects are included in the studies. Lattice vacancies introduced by quenching or irradiation with electrons are studied through their influence on the oxidation properties of the graphite surfaces. Vacancy motion is studied by self-diffusion techniques and by annealing studies of the oxidation properties. Electron microscopy of oxidation pitting at point defects or clusters of point defects in surface planes are also studied. Magnetoresistance changes as a function of vacancy concentration is under study. Vacancy studies are correlated with fast neutron effects in graphite.

Screw and edge dislocations are studied in natural single crystals by electron microscopy and correlations of these observations with visible spiral markings on some crystals implies a screw dislocation mechanism of crystal growth. The influence of the strained region around screw dislocations on the chemical reactivity is under study. Edge dislocations are observed by direct transmission on thin cleavage flakes. Edge dislocations are not present in carefully handled crystals but appear under slight mechanical deformation.

The surface reactions of graphite crystals with various oxidiants such as O_2, CO_2, H_2O, etc., under various conditions and in the presence of absorbed molecules or with metallic catalysts are under detailed study. Similarly, the lamellar reactions of graphite with a wide variety of chemicals continue to be of great interest. A recent example is the reaction of $InCl_3$-Cl_2-graphite in which $InCl_3$ reacts with graphite in the presence of Cl_2 to form an interlamellar compound.

Contractor: Brookhaven National Laboratory, Associated Universities, Inc. Upton, Long Island, New York

Contract: AT(30-2)-Gen-16

Brief Title: GRAPHITE BONDING STUDIES

Investigators: D. R. Schweitzer and D. H. Gurinsky

Scope of Work

The objective of this work is to determine the effect of different experimental parameters on the degree of trigonal, tetrahedral and unsaturated bond formation in carbons and graphites. The studies will be made in neutron and gamma fields and in the absence of radiation. Changes in the nature of bond formation in graphites under mechanical and thermal stresses in strong magnetic fields will also be investigated. An attempt will be made to follow the diamond to graphite conversion with temperature by magnetic susceptibility and electron spin resonance measurements.

The effect of hydrogen and methane on the formation of bonds between single crystals of graphite are under study. The effects of catalysts on bond formation in graphites and the mechanisms of these reactions are being investigated.

Contractor: Columbia University, New York, New York

Contract: AT(30-1)-1593

Brief Title: A STUDY OF INCLUSIONS IN URANIUM

Investigators: George L. Kehl

Scope of Work

The above captioned research is a continuation of a study pertaining to the transformation kinetics of selected inclusions in uranium as a function of time and temperature. Of particular interest are the changes in UC, U(C,N), UN, and so-called UO inclusions, when held at temperatures of 810°C and 1090°C for times up to 3600 and 500 hours respectively. After varying times at the two temperatures, dimensional changes of the inclusions are determined, and changes in composition are noted by hardness measurements of the inclusions proper, x-ray diffraction analyses, darkening characteristics in 1:1 nitric acid-water reagent, air oxidation characteristics, and the reception of the inclusion to an electrodeposit of copper. Confirming data are being obtained that support an earlier observation that the isothermal solution of most inclusions is exceedingly slow, and that U(C,N) eventually transforms to UN, and so-called UO to UC.

Contractor: Emmanuel Missionary College, Berrien Springs, Michigan

Contract: AT(11-1)-972

Brief Title: MECHANICAL PROPERTIES OF SEPARATED METALLIC ISOTOPES

Investigators: Donald D. Snyder

Scope of Work

Research in this project involves the measurement of certain of the mechanical and thermal properties of separated stable isotopes. The immediate program is the extension of previous measurements of the elastic modulus of isotopically enriched samples of lithium to lower temperatures and to measure their temperature coefficients of linear expansion. The objective of the study, besides furnishing basic physical data on an important class of substances, is the testing and possible extension of theories of the solid state. The isotopes of a single element provide a set of closely related substances which differ significantly (insofar as this study is concerned) only in atomic mass. This parameter then serves as a probe for testing theoretical predictions of certain of their physical properties.

The temperature range of the study will be from room temperature to liquid-nitrogen temperature.

Contractor: Michigan State University, East Lansing, Michigan

Contract: AT(11-1)-400

Brief Title: THERMAL PROPERTIES OF SEPARATED METALLIC ISOTOPES

Investigators: D. J. Montgomery

Scope of Work

As part of a program investigating phase changes with the aid of isotopic mass as a probe, the viscosity of separated lithium isotopes was measured near the melting point. The results suggested that the viscosity of simple molten metals depends on temperature in a more simple manner than does that of complicated liquids, such as hydrocarbons. Accordingly it is proposed to study with increased precision the viscosity of Li-6 and Li-7 over wider temperature ranges, to determine with high precision the exactness of the laws relating viscosity to temperature.

To study phase changes themselves, the effect of isotopic composition on melting and freezing points will be studied by determining the phase-equilibrium diagrams for lithium hydride made from different proportions of lithium-6 and lithium-7, hydrogen-1 and hydrogen-2. The study can then be extended to lithium halides and to other properties.

Contractor: Oklahoma, University of, Norman, Oklahoma

Contract: AT-(40-1)-2570

Brief Title: INFLUENCE OF HYDROGEN ON THE MECHANICAL PROPERTIES OF METALS

Investigators: Raymond D. Daniels

Scope of Work

This project is a study of the influence of hydrogen on the mechanical properties of metals. The objective of this research is to obtain significant data on the embrittlement phenomena associated with the presence of hydrogen in metals, and thereby to gain an improved understanding of these phenomena and the mechanisms involved.

Investigation of the columbium-hydrogen system will be continued along the following lines:

(1) Columbium-hydrogen alloys will be prepared by thermal equilibrium techniques.

(2) Hydrogen diffusivity in columbium will be determined over a range of temperatues and as a function of prior cold work.

(3) The mechanical properties of hydrogenated columbium will be studied and embrittlement phenomena evaluated.

(4) Certain high strength columbium alloys will be included in this investigation to determine their sensitivity to the presence of hydrogen.

Contractor: Pennsylvania State University
University Park, Pennsylvania

Contract: AT(30-1)-2581

Brief Title: FUNDAMENTAL STUDIES IN HIGH-TEMPERATURE MATERIALS PHENOMENA

Investigators: M. E. Bell, R. Roy, C. Crowe, and G. W. Brindley

Scope of Work

Scope 1 - High Temperature-Pressure Physical Property Measurements.

The first six to eight months of operation were devoted to assembling various types of electrical and magnetic measurement equipment in a new laboratory. Initial emphasis has been on the measurement of dielectric constant and loss in relatively small samples over a wide range of frequencies, and on the training of technician and graduate student personnel in conducting and interpreting these measurements. Sample holders have been designed and built for work from liquid nitrogen temperature to 400°C; and techniques developed for maximum exploitation of powder samples by pressing to theoretical density. A 100-ton high pressure assembly for subjecting 3/8" diameter samples up to 100,000 atmospheres pressure during measurements has been constructed. Suitable hot-air furnaces have been set up for heating samples during electrical measurements.

Phases on which evaluations have already been started include the CaF_2-YF_3, $MgAl_2O_4$-Al_2O_3, and ZrO_2-CaO systems, all with "massive" concentrations of chemically introduced defects whose influence on the electrical properties is being investigated; slightly reduced TiO_2, in which the nature of the defects is under study as a function of the partial pressure of O_2; and the system Ag_2S-PbS-Bi_2S_3 in which resistivity changes are being observed at very high pressures as a function of defect type.

Scope II - Electrical Resistivity Measurements of Materials in Relation to High Temperature Transformations.

Resistance measuring equipment has been assembled covering resistivities from 10^{16} ohm-cm to 10^{-6} ohm-cm in three ranges. Actual research on this scope has been delayed due to Prof. Brindley's absence on sabbatical leave. Active research will begin about September 1, 1961.

Contractor: Virginia Polytechnic Institute

Contract: AT-(40-1)-2689

Brief Title: THE RESISTIVITY AND MAGNETIC SUSCEPTIBILITY, THE HALL EFFECT AND SPECIFIC HEAT OF CERIUM AS DETERMINED BY ITS TEMPERATURE DEPENDENT CRYSTAL STRUCTURE

Investigators: T. E. Leinhardt

Scope of Work:

Measurements will be made of the temperature and crystal structure dependence of the electrical resistivity, magnetic susceptibility, Hall Effect, and specific heat of pure cerium metal. An attempt will be made to explain anomalies in the properties in terms of changes of crystal structure in cerium. A study will be undertaken to determine the feasibility of using resistance measurements to infer crystal structure. The results will be interpreted in terms of current theory and findings of other investigators.

Section II

PHYSICAL RESEARCH IN THE NATURE OF MATTER

I-A

Atomic and Electronic Structure of Materials; Alloy Theory

Contractor: Argonne National Laboratory, Lemont, Illinois

Contract: W31-109-eng-38

Brief Title: ALLOY THEORY OF THE TRANSITION ELEMENTS

Investigators: A. T. Aldred, J. B. Darby, Jr., A. E. Dwight, D. J. Lam, M. V. Nevitt, D. O. VanOstenburg

Scope of Work

This research effort is directed to the interpretation of the occurrence and properties of solid solutions and intermetallic compounds in terms of the electronic structure of the component elements and the electronic interactions that occur upon alloying. The following aspects of this problem are under study:

Scope I The Crystal Chemistry of Intermediate Phases

An extensive experimental survey has been made of the occurrence of intermediate phases in binary and ternary systems involving metals of the three long periods, of the lanthanide series, and of the actinide series. Over one hundred and twenty compounds not previously reported in the literature have been found during the course of the survey. The major share of these phases have been identified crystallographically as having structures of the following types: Cr_3O-type (beta-tungsten), Ti_2Ni-type, Si_2Mo-type, Al_2Cu-type, CsCl-type, $MgCu_2$-type, $MgZn_2$-type, $TiNi_3$-type, $TiAl_3$-type, $TiCu_3$-type, $AuCu_3$-type, $CaCu_5$-type, αMn and sigma. The phases have been classified in terms of their characteristic stoichiometric ratios as well as their structure types. The major families that result from this classification are being systematically analyzed to learn how atomic size and valency effects are influential in determining which structure will occur. When several families of compounds have been found at the same stoichiometric ratio they have been examined for the presence of structural similarities.

Scope II Magnetic Properties of Intermediate Phases and Solid Solutions

Saturation magnetic moment measurements have been made on alloys of iron in order to clarify the nature of the electronic states that exist in certain intermediate phases and solid solutions. A study of the CsCl-type phase TiFe indicated that in this compound the unpaired d electrons on the Fe atom have been redistributed in such a manner as to leave no uncompensated spins except in regions of disorder in the lattice. In constrast to this behavior, the equiatomic V-Fe alloy with CsCl-type long range order was found to be ferromagnetic with a moment on the Fe atom of 0.82 Bohr magnetons. This indicates that when Fe is paired with V in the CsCl-type structure it donates a smaller number of its ferromagnetic electrons to bonding than when Ti is its partner.

Measurement of the magnetic moments of V-Fe alloys over a range of composition has demonstrated that for a given composition the net unbalance of spins in the magnetic d-band of Fe is dependent upon the crystalline environment. The

Fe moment is highest for the disordered body-centered cubic structure. It is decreased by about 20 pct by Cs-Cl-type ordering, and is lowered by a factor of three by the transformation to the sigma phase.

The scope of the magnetic properties research is now being broadened to include measurements of paramagnetic susceptibility of solid solutions having Pauli paramagnetism and of compounds and solid solutions characterized by localized moments. Polycrystal and single crystal studies will be made. In conjunction with nuclear magnetic resonance measurements (Scope IV), a clearer picture of the metallic binding can be achieved.

Scope III Calorimetric Studies of Intermetallic Compounds of Transition Elements

A new portion of the alloy theory program is devoted to the measurement of the heat of formation of intermetallic compounds and solid solutions involving transition metals of the first long period. A twin liquid-metal solution calorimeter operable at high temperature, is now being assembled for this purpose. The necessary preliminary data relating to the solubilities and the kinetics of dissolution of first long period elements in certain liquid metal solvents is now being collected.

Scope IV Nuclear Magnetic Resonance Studies in Alloys

A study of alloys through the technique of nuclear magnetic resonance is also under investigation for the determination of their electronic and structural properties.

Knight shift measurements in alloys is of exceptional importance because it is determined in part by the electron density and wave functions in the material. Our study of this parameter versus composition allows a determination of the Fermi surface as well as the electronic wave function character in alloys.

Of equal importance is the study of the quadrupole effects of foreign atoms in solid solution. This work in connection with theoretical models enables us to speculate on the distribution of solute atoms and other related problems. Nuclear magnetic resonance experiments augmented with other techniques such as magnetic susceptibility, electronic specific heat, etc., gives us an independent measurement, the results of which must be in harmony with a correct theory of alloys.

Currently, we are applying resonance techniques to many of the alloy systems previously mentioned in this summary in order to obtain as much information as possible regarding the general theory of alloys.

Contractor: Argonne National Laboratory, Lemont, Illinois

Contract: W31-109-eng-38

Brief Title: X-RAY AND NEUTRON DIFFRACTION STUDIES

Investigators: D. S. Flikkema, L. Heaton, M. H. Mueller, N. S. S. Murthy
S. S. Sidhu

Scope of Work

This research work is concerned with the use of neutron and x-ray diffraction techniques in the study of problems in the field of crystallography, magnetic structure, and the liquid state.

Recent neutron diffraction instrumentation has involved the completion of the basic horizontal neutron spectrometer together with initial alignment and debugging.

At the present time, necessary supplementary equipment is being added to the basic instrument in order to permit the use of the instrument for the study of crystal dynamics involving a change of neutron energy. A smaller scale neutron diffraction instrument, especially suitable for single crystals, is also being assembled using the same primary neutron beam as used for the horizontal instrument mentioned above. Since its counter arm will travel in a vertical direction, it will be possible to use both instruments at the same time.

Recent neutron and X-ray diffraction studies are:

(1) A nuclear null-matrix has been used to assist in the study of the magnetic structure in manganese-cobalt carbides and also in copper-manganese alloys.

(2) The crystal structure of $CuTi_2$ has been worked out from neutron diffraction data indicating that the unit cell is three times as large as the X-ray data seem to indicate.

(3) A single crystal neutron diffraction study of disodium tetranitronitrosohydroxyruthenate (III) 2 hydrate has been started. To date only a very preliminary structure has been worked out for a part of the atoms. The neutron diffraction data for over 1400 reflections should now permit the refinement of the structure and the location of the light atoms including the hydrogens.

(4) A determination of the neutron coherent scattering amplitude of K^{39} and Rb^{85} has been carried out together with a recheck of the values for the normal isotopic mixtures of K and Rb. Current work is also being carried out for several Zr isotopes.

(5) The angular distribution of neutrons scattered by krypton in the liquid state at various temperatures from 117°K to 210°K was carried out. By use of a sample cell fabricated from a single aluminum crystal, it was possible to

obtain diffraction patterns up to the critical temperature and pressure. The number of nearest neighbors was calculated from the radial atomic distribution function.

(6) A comparison of precise lattice parameters from Bell Laboratories for alpha uranium single crystals with our results obtain from polycrystalline material indicates that there is probably very little significant difference. Some preliminary results on the determination of the atomic positional parameter, y, as a function of temperature has indicted a rather small change at least up to 500°C.

(7) Some further modification of the precision lattice parameter computer program has been made, and this program has been shared with a number of other laboratories for use on the IBM-704 computer.

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

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

Brief Title: ELECTRONIC STRUCTURES OF METALS AND ALLOYS

Investigators: T. G. Berlincourt, R. R. Hake, D. H. Leslie, A. C. Thorsen, and W. J. Tomasch

Scope of Work

This project is concerned with studies of properties which can be directly related to the electronic character of metals, emphasis being placed upon transition and actinide 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 low temperature specific heat studies. The latter measurements reveal 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 electrical resistivity, magnetoresistivity, Hall effect, and superconductivity are also used to characterize the electronic structure. By inter-relation and interpretation of the experimental results in terms of electronic energy band theory, attempts are made to form a coherent picture of the electronic structure in metals and the way in which this is affected by alloying additions.

Recent progress on this project has been marked by (1) the first successful observations of the de Haas-van Alphen effect in Ca, K, and Re, (2) clarification of the nature of the electronic structure of metastable body-centered-cubic transition metal alloys, (3) illucidation of the role of dilute magnetic impurities in Ti, and (4) discovery of high current density, high magnetic field superconductivity in the alloy system Nb-Zr.

Contractor: Brookhaven National Laboratory, Associated Universities, Inc., Upton, Long Island, New York

Contract: AT(30-2)-Gen-16

Brief Title: NEUTRON DIFFRACTION RESEARCH

Investigators: G. J. Dienes, B. C. Frazer, R. Nathans, H. Danner, G. H. Vineyard, P. J. Brown, H. Boutin, H. A. Alperin, S. J. Pickart

Scope of Work

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.

Studies of Magnetic Materials

The magnetic properties of a class of inorganic compounds with the orthorhombic chemical structure of $CrVO_4$ have been investigated. The magnetic structure of $CrVO_4$ is formed from alternating ferromagnetic sheets of Cr^{3+} ions on the (002) planes, but the ions in some of the sulfates, for example, are coupled antiferromagnetically in the (002) planes. The Fe^{2+} and Ni^{2+} ions have their spins oriented parallel to [010] with ferromagnetic coupling between successive (002) sheets while $CoSO_4$ does not have a single spin axis. The moments found for Fe^{2+}, Ni^{2+}, and Co^{2+} all agree very well with the expected values, but the Cr^{3+} moment seems to be somewhat lower than expected.

As a further extension of the work on neutron form factors the spatial distribution of the magnetic electrons in magnetite has been studied with polarized neutrons. Of particular interest here are the differences which were observed between the form factor of the iron atoms on the tetrahedral sites and those on the octahedral sites (the former are entirely Fe^{3+} atoms while the latter are a mixture of Fe^{3+} and Fe^{2+} atoms). The differences in form factors are probably due to the difference in the coordination of the surrounding oxygen atoms. The data also showed that the magnetic electrons for the Fe^{3+} atoms on the tetrahedral sites, which in this case form the full complement of the 3d electrons, are not spherically symmetric.

Another important area of study is that of magnetic alloys in which the moment of the component transition element deviates from its value in the pure metal. As an example of this field, polarized beam measurements on Fe_3Al have reached the point where meaningful Fourier projections of the magnetic electron density can be made. These projections demonstrate clearly and unambiguously the movement of magnetic electrons into bonds and the difference in the aspericity of the magnetic electrons on the two different iron sites.

Studies of Non-Magnetic Solids

The tetragonal structure of ferroelectric $BaTiO_3$ has been re-examined by applying the completely general method of least squares refinement in IBM 704 calculations. While it appears that the previously reported structure is nearly correct, it was found that the solution of the problem, using the old (h0l) data, is limited by "interaction" between certain parameters. The interaction apparently breaks down if a sufficient number of (hhl) data are included in the refinement. A set of such data has been collected, and it is hoped that an unambiguous solution will now be possible. The results of this study illustrate very clearly the pitfalls, some ignored in the past, involved in the study of pseudo-symmetric structures. Since all ferroelectric structures are pseudo-symmetric, the accuracy of a number of such structures in the literature is open to some question.

A study of the structural changes in the ferroelectric transition of $NaNO_2$ is nearly finished. A very accurate structure for the ferroelectric phase was reported last year. The structure above the Curie point has proved to be more intricate than anticipated. A fully rotating model has been eliminated and it seems likely that a proper model is one that can either be considered in terms of the simple disordered model with a considerable degree of libration of the NO_2 groups, or as involving hindered rotation with a rather high barrier.

The principal ferroelectric structure to be investigated next is that of $LiH_3(SeO_3)_2$, but certain other studies are also planned. Among the latter is an investigation of damage to Rochelle salt by ionizing radiation. It has been known for some time that x-rays and γ-rays produce drastic changes in the dielectric properties of this crystal, and an explanation has been offered involving locking of the ferroelectric domains by trapped damage products. An alternate explanation could be that the damage products actually knock out the ferroelectric phase by rendering the monoclinic structure unstable. This can be checked conclusively by neutron diffraction measurements.

Order-Disorder Transformations

The diffuse scattering of monochromatic neutrons from a single crystal of β-brass, isotopically enriched in Cu^{65}, has been measured at three temperatures above the critical temperature in both the $\lfloor 100 \rfloor$ and $\lfloor 111 \rfloor$ directions. The short range order parameters obtained from the least square analysis of the data are a quantitative measure of both the degree and extent of the local order. From the combined $\lfloor 100 \rfloor$ and $\lfloor 111 \rfloor$ data it is theoretically possible to solve for 23 short range order parameters. In most systems measured to date the local order has been found vanishingly small for atoms which are more than 5 to 10 neighbors apart. This is not the case for β-brass, and the most important result to date is the finding that the local order in this material is correlated over much larger distances than usually pictured. The same techniques are now being applied to isotopically enriched α-brass.

Liquids

Recent work on liquids has been primarily theoretical. Previous theoretical work has been extended in two directions:

1. The Born-Green method has been generalized to the case of distribution functions involving two times.

2. An application of the law of corresponding states to the scattering of neutrons and x-rays from a fluid has been developed.

Contractor: (The) Catholic University of America, Washington, D.C.

Contract:

Brief Title: ULTRASONIC STUDIES OF ALKALI METALS

Investigators: Paul H. E. Meijer

Scope of Work

This project consists of studies of the electronic structure of metals with specific emphasis on definition of the Fermi surfaces of alkali metals. High purity metal crystals will be grown and the Fermi surfaces studied using magneto-acoustic techniques with equipment already on hand and magneto-resistance with equipment to be developed.

Theoretical research includes further study pertaining to the electronic structure of metals, particularly the directional dependence of relaxation time and mean free path. Lattice-lattice and spin lattice relaxation also will be investigated.

Contractor: Franklin Institute, Philadelphia, Pennsylvania

Contract:

Brief Title: X-RAY INVESTIGATION OF THE STRUCTURE OF SMALL PARTICLES

Investigators: Heinz G. F. Wilsdorf and F. R. L. Schoning

Scope of Work

This research has as its subject the study by x-ray techniques of the structure of small particles. The principal objective of the work is to separate line broadening caused by lattice strain from the diffraction effects caused by small particles. An evaporation method will be used to produce small particles. Careful measurements of the shape of the diffraction profile will then be followed by Fourier analysis in an attempt to characterize quantitatively the difference in lattice parameter between the surface and the interior of crystals.

Contractor: Temple University, Philadelphia, Pennsylvania

Contract:

Brief Title: STUDY OF THE IB-IIB BETA PHASE ALLOYS

Investigators: Leonard Muldawer and H. Amar

Scope of Work

The research effort on this program is directed to the study of the structures of intermetallic compounds between IB and IIB metals. Emphasis will be placed on beta phase structures found in binary and ternary combinations of these systems. Work will involve first structural determinations and study of ordering and transformation reactions in $AgAuCd_2$ and $AgAuZn_2$. Martensitic reactions in AgZn also will be investigated. An attempt will be made to clarify the electronic structures of these phases by spectral reflectivity studies.

Contractor: Mellon Institute, Pittsburgh, Pa.

Contract: AT(30-1)-2684 - Mellon Institute

Brief Title: ALLOYS OF THE NOBLE METALS

Investigators: T. B. Massalski

Scope of Work

Certain aspects of the relationship between the electronic structure, phase stability and physical properties of alloy phases are being studied experimentally; and a portion of this work also will be discussed in a review article.

Lattice spacings of some Cu-based and Ag-based close-packed hexagonal intermediate phases will be measured accurately at room temperature and discussed in terms of possible interactions between the Fermi surface and the Brillouin zone. This research will follow previous work in this field which is already published or about to be published.

The stacking fault probability, following deformation by filing, will be measured in a series of alloys in the α phase of the Ag-Cd system. As far as possible strict experimental conditions, regarding temperature of filing and mode of filing, will be maintained. The obtained data will be discussed in terms of possible changes in the stacking fault energy, dislocation density and electronic structure.

Phase stability, order-disorder, and phase relationships in the Cu-Ga system will be studied by dilatometric, micrographic and x-ray techniques as a preliminary groundwork to the study of the massive transformation in these alloys. Some aspect of phase transformations in the β-phase region of the Ag-Zn system will also be studied.

Contractor: Pennsylvania State University, University, Park, Pa.

Contract: AT(30-1)-1516

Brief Title: X-RAY AND NEUTRON ANALYSES OF STRUCTURAL MECHANISMS FOR PHYSICAL PROPERTIES OF CRYSTALS

Investigators: Ray Pepinsky

Scope of Work

The primary goal of this research is the determination of crystal-structural mechanisms for spontaneous polarization and its field-reversability in ferroelectric crystals. Both x-ray and neutron diffraction methods are employed, the latter through use of the Brookhaven reactor. A new x-ray technique, involving synchronous pulsing of a grid-controlled x-ray source, at controllable phases with respect to a polarizing square-wave voltage signal applied to the ferroelectric crystal, and with variation in frequency from dc to 50,000 cys, is applied in order to determine the time-characteristics of structure alteration with field. The method depends on anomalous x-ray scattering for indication of the reversal of polarization axis; the absolute configuration of the structure is automatically obtained.

Structure analyses of certain crystals of special interest to Brookhaven scientists also is in progress.

Research on crystal-preparative techniques, and growth of materials for dielectric, x-ray and neutron studies is continuing.

Improved crystallographic computing programs for the 704 and 7090 machines at the AEC-New York University Computing Center also are being developed.

Contractor: Pittsburgh, University of, Pittsburgh, Pennsylvania

Contract: AT(30-1)-2163

Brief Title: CALORIMETRIC, STRUCTURAL AND MAGNETIC STUDIES OF METALS AND INTERMETALLIC COMPOUNDS

Investigators: R. S. Craig

Scope of Work

The following problems have been designated for investigation under this contract during the current fiscal year:

1) A study of the Long Range Order Parameter in Mg_3Cd and $MgCd_3$.

2) A study of structures and magnetic properties of solid solutions based on Gadolinium.

3) Measurement of the specific heats of dilute solid solutions of Mg and Cd in the liquid helium temperature range.

4) A study of the specific heats of alloys of the pseudo-binary systems $TiFe_{2-x}Co_x$, $TiFe_{2-x}Ni_x$ and $TiFe_{2-x}Cu_x$ in the liquid helium temperature range.

5) A study of the specific heat of β-manganese between 20 and 300°K.

6) An investigation of phenomena at temperatures below 1°K. This project calls for the construction of a cryostat employing He^3 as the refrigerating liquid. $MgCu_2$ has been designated as the first material to be studied at the lower temperatures.

Contractor: Union Carbide Nuclear Company, Oak Ridge National Laboratory, Oak Ridge, Tennessee

Contract: W-7405-eng-26

Brief Title: ALLOY THEORY RESEARCH

Investigators: J. O. Betterton and G. D. Kneip

Scope of Work

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. Investigations of phase diagrams, low-temperature electronic and lattice specific heats, electrical resistivity and magnetoresistivity, magnetothermal effects, the transition temperature of superconductivity, and high-temperature thermodynamic properties by means of vapor pressures are all used to investigate both the alloying process and electronic structure of metals and alloys. Studies to date have concerned mostly zirconium, but in the field of transport properties at least this work will be extended to high-purity Groups V-A and VI-A single crystals

Contractor: Union Carbide Nuclear Company, Oak Ridge National Laboratory, Oak Ridge, Tennessee

Contract: W-7405-eng-26

Brief Title: X-RAY DIFFRACTION RESEARCH

Investigators: H. L. Yakel, B. S. Borie and C. J. Sparks

Scope of Work

Scope I. Structural Studies

An investigation of structural changes occurring near the order-disorder transition in nonstoichiometric copper-gold alloys is in progress in an effort (1) to determine the extent to which such transitions follow classical thermodynamic rules and (2) to study the detailed structure of the anti-phased structure formed as an intermediate in the ordering process. High-temperature x-ray diffraction powder techniques are employed to avoid uncertainties due to quenching conditions.

Aging transformation of metastable body-centered cubic alloys are being studied with the aid of single-crystal x-ray diffraction techniques. The effect of neutron irradiation on the transitions of zirconium-15 at. % niobium alloys is currently under examination. Single-crystal diffraction patterns of uranium-30 at. % molybdenum alloys, heat treated to produce the γ' configuration, have shown that the C11b($MoSi_2$) structure proposed for the ordered state is not correct in detail. Additional work is in progress to determine a more accurate structure for this phase. Efforts to retain a body-centered cubic structure by rapid quenching in other alloy systems have suggested that quench-induced transitions may occur, as for example in the uranium-niobium system, with critical dependence on the quenching conditions. Further studies of these transitions are proposed.

Structural investigations in mixed oxide systems have been given added impetus by the discovery of new simple mixed oxide compounds containing BeO. Work is currently in progress on two compounds, $Ca_2Be_3O_5$ and $Sr_2Be_3O_5$. While these materials apparently have the same chemical formula, x-ray diffraction data from polycrystalline and single-crystal specimens show large structural differences between them. A complete determination and refinement of the crystal structure of $LuMnO_3$, a representative of a new class of ABO_3 compounds, has been completed to the extent that a novel fivefold co-ordination of manganese atoms has been confirmed.

Scope II. Studies of Crystalline Imperfections

Deviations from perfect periodicity in the crystal lattice may be detected by x-ray diffraction either by measurements of diffuse scattering, or by measurements of the shapes of the Bragg reflections, depending on the nature of the imperfection. Both types of experiments are currently being carried out.

An x-ray diffractometer has been designed and constructed which is capable of automatically measuring the distribution of diffuse scattering in a plane of reciprocal space. This instrument is currently being used to determine in detail the short range structure of the alloy copper-16 at. % aluminum. It is intended to measure the effect of reactor radiation on the short range structure of this material.

Techniques have been developed which allow the detection of the Bragg maxima of oxide films grown on metals when they are as thin as 100 A. Studies of the shapes of these broadened peaks have been interpreted quantitatively in terms of the thickness of the film and the strain in the film. These measurements have led to a better understanding of how the structure of an oxide film changes as it grows.

Contractor: Virginia Polytechnic Institute, Blacksburg, Virginia

Contract: AT(40-1)-2564

Brief Title: FACTORS GOVERNING THE FORMATION OF Cr_3O-TYPE STRUCTURES

Investigators: John F. Eckel

Scope of Work

The primary aim of this program is to study the factors governing the formation of the Cr_3O-type structure in systems containing transition elements. A critical examination will be made of the importance of atomic size effects and electronic interactions in controlling formation of this structure.

During the past year equipment has been assembled for specimen preparation and for high-temperature x-ray diffraction. The investigation of structure of alloys in the Cr-Si-Sn, V-Rh-Si, Nb-Rh-Si, and V-Si-Sn system has been continued.

Contractor: Wisconsin, University of

Contract: AT(11-1)-987

Brief Title: BRILLOUIN ZONE STRUCTURES OF ALUMINUM ALLOYS

Investigators: Richard A. Dodd

Scope of Work

The purpose of this work is to attempt a contribution to the theory of alloys by making various physical measurements on polycrystal and single crystal binary aluminum alloys, and interpreting the results in terms of Brillouin zone structures of the alloys.

The initial phase of the work involves a comparison of the theoretical (x-ray) and immersion densities of aluminum-magnesium, aluminum-zinc, and aluminum-silver alloys. The compositions investigated will range up to approaching the limit of solid solubility, so that quenched alloys will be used for both the immersion densities and for the lattice parameter measurements. This preliminary work is a check on the work of Ellwood (Jnl. Inst. Metals, 1952/53) who reported discrepancies in immersion and x-ray densities which he interpreted as being due to vacant lattice sites. These in turn were interpreted in terms of the Brillouin zone structure of aluminum. We tend to doubt Ellwood's results, and consider that a check of his work constitutes a necessary preliminary to this investigation.

The second, and final, phase of the investigation will involve the measurement and interpretation of aluminum solid solution single crystal eleastic constants. The work during this first year will be mostly concerned with the setting up of ultrasonic pulse echo equipment, and with the growth of high alloy solid solution single crystals. Diffusion methods of crystal preparation will be investigated.

Section II-B

Imperfections, Microstructure, and Related Phenomena

Contractor: Arizona, University of, Tucson, Arizona

Contract:

Brief Title: THE FREQUENCY OF ANNEALING TWINS

Investigators: Daniel J. Murphy

Scope of Work

The object of this research is to provide fundamental information concerning the origin and behaviour of annealing twins. Specific goals of the program include the following:

(a) Determination of the frequency of annealing twins as a function of grain size.

(b) Study of how the number of twins varies during grain growth.

(c) Examination of the effect of solute elements on twin formation and disappearance.

(d) Measurement of the activation energy for movement of an incoherent twin boundary.

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

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

Brief Title: DEFECT-CONTROLLED PROCESSES IN METALS AND ALLOYS

Investigators: A. Sosin and C. J. Meechan

Scope of Work

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 program may be classified into three parts.

a) A study of vacancy characteristics in a pure metal lattice. Diffusion in a large thermal gradient has been observed in gold and copper, using inert markers as guides. The direction of motion in these two systems is opposite, implying the vacancy formation energy is more than the migration energy in one material and less in the other. Direct visual evidence for this interpretation has also been obtained.

b) A study of vacancy characteristics in a slightly doped metal and the nature of the vacancy-dopant interaction. Quenching and high temperature equilibrium measurements of aluminum with small amounts of additions have been made and are in progress.

c) Effect of vacancies on segregation and precipitation, as revealed by electrical resistivity measurements, electron microscopy, and X-ray diffraction.

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

Contract: W-7405-eng-48

Brief Title: RATE CONTROLLING DEFORMATION MECHANISMS IN METALS AND ALLOYS

Investigators: John E. Dorn

Scope of Work

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, energetics of lattice imperfections, electronic energies, solution theory, diffusion, short range order, long range order, kinetics of reactions, etc. In fact, practically every basic concept of the physics and chemistry of alloys is involved in 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.

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

Contract: W-7405-eng-48

Brief Title: PHYSICAL CERAMIC RESEARCH

Investigators: R. M. Fulrath

Scope of Work

The purpose of this research is to increase the fundamental understanding of those factors which influence the mechanical properties of polycrystalline, single crystalline, and multiphase inorganic nonmetallics.

A significant portion of the investigation is concerned with the development of microscopic internal stresses in multiphase ceramics where the thermal expansion mismatch occurs. Model systems of crystals dispersed in a glassy phase are being used in this study area. Other factors which influence the mechanical strength, such as particle size and shape, volume fraction of dispersed phase, and porosity, are also being investigated.

It is becoming apparent that an interface between phases or a grain boundary in ceramics may show varying degrees of continuity or interfacial bonding. This is reflected in the mechanical strength of the material. Wetting of the crystal by the glass used in model systems has indicated that this factor is of extreme importance. Studies of wetting and the effect of grain boundary continuity in polycrystalline ceramics are currently in progress.

Also under investigation are the reaction heats developed in ceramic materials, since these heats produce thermal gradients and lead to macroscopic body stresses during the firing process.

Contractor: California, University of, Berkeley, California

Contract: AT(11-1)-34, Proj. #62

Brief Title: DISPERSED PHASES

Investigators: Lawrence Himmel

Scope of Work

This study is concerned with the influence which finely-dispersed particles of a second phase exert on the properties of metals and alloys. Using a variety of techniques, including thin film microscopy, efforts are being made to establish the manner in which the presence of the dispersed phase modifies the deformation behavior of the matrix as well as its subsequent response to heat treatment. The materials under investigation consist of oxide particles dispersed in a silver or copper matrix; these materials are prepared by internal oxidation of dilute solid solution alloys.

Dislocation damping measurements are being made over a wide range of temperatures in order to determine the effectiveness of oxide dispersions as pinning points for dislocations in silver. A study is also being made of Bordoni damping in internally-oxidized silver alloys. Other problems under investigation include:

1. A study of the effect of oxygen and other elements in solid solution on the stacking fault energy of silver.

2. A study of the effectiveness of oxide dispersions as sinks for vacancies in quenched alloys.

3. A study of the influence of oxide dispersions on the development of Kirkendall-type porosity associated with diffusion processes in alloys.

4. A comparison study of the mode of deformation of high-purity silver and internally-oxidized silver alloys.

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

Contract: W-7405-eng-48

Brief Title: THEORETICAL AND EXPERIMENTAL PROPERTIES OF MATERIALS

Investigators: Earl R. Parker

Scope of Work

The primary objective of the research in progress is to conduct experiments that will elucidate the anomalous mechanical behavior of iron at low temperatures. At liquid nitrogen temperature and below, the yield strength of iron increases at an abnormally rapid rate. There is no reasonable explanation for this behavior at the present time. It is suspected that this behavior is due to the presence of interstitial atoms which react with dislocations and cause the rapid increase in yield strength as the temperature is lowered. Some ultrahigh purity iron has been obtained and will be used for the purpose of determining the effect of impurities on the temperature dependence of the yield strength. In addition, the internal friction characteristics of the ultrahigh purity iron are to be determined by means of Bordoni-type experiments. Subsequent to the evaluation of the high purity iron, carbon and nitrogen will be introduced in known concentrations and the internal friction will be determined to evaluate the role played by these interstitial elements.

In addition, work is continuing on studies of the cause of solution hardening. Techniques have been developed to the extent that it has now become possible to measure changes in grain boundary energy produced by alloying elements at room temperature. Also, a small effort will be devoted to fundamental investigations concerned with flow and fracture processes in nonmetallic crystals.

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

Contract: W-7405-eng-48

Brief Title: CERAMIC MICROSTRUCTURES AND HIGH TEMPERATURE REACTIONS

Investigations: J. A. Pask

Scope of Work

The over-all scope of this project is a study of the factors responsible for the development and control of microstructure of ceramic bodies (in this case, essentially oxides), and the correlation of the microstructures with the mechanical behavior of such bodies. Model systems of halides are frequently used because of their lower melting temperatures. One of the principal areas of study in connection with this objective is that of solid state reactions. Such studies include measurement of diffusion rates, and determination of the nature of the mechanisms and the kinetics of such reactions involving single crystals and powders. Another facet involves a study of the nature and control of surface and interfacial characteristics. Wetting, adherence, and grain boundary structures are largely dependent upon such factors. These factors and others, such as impurities and crystal defects, become important in sintering studies whose objective is to obtain a particular microstructure. Search for other factors affecting sintering is also an objective of the studies. The mechanical properties associated with the plastic behavior of single crystal and polycrystalline specimens are of fundamental interest in the over-all problem.

In addition, the nature of the stress-strain curves in compression and bending and creep in compression at a range of temperatures up to 1600°C are being investigated and interpreted in terms of microstructure. The areas of study are of particular value in obtaining a fundamental understanding of physical ceramics.

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

Contract: W-7405-eng-48

Brief Title: ELECTRON MICROSCOPE STUDIES OF THE MICROSTRUCTURE OF CRYSTALLINE MATERIALS

Investigators: G. Thomas

Scope of Work

The over-all object of the use of transmission electron microscopy allied with other techniques is to gain a better understanding of the relationship between the microstructure of materials and their properties. The work is at present aimed towards mechanical properties, but this will be extended in the near future to include investigations of the effects of radiation damage on the structure and properties of metals and alloys. Since the mechanical properties depend on the nature and distribution of defects and second phases, many of which cannot be seen without using electron microscope 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 metals is currently underway with molybdenum, and will be extended to include work on vanadium, tantalum, tungsten and columbium. At present, the ceramics work is confined to MgO crystals. Additional work will include studies of vacancies in metals and alloys using copper base materials, precipitation-hardened systems (Cu-Be series of alloys, martensitic alloys), etc.

The program is designed so as to indicate means of improving the properties of materials already available whilst at the same time utilizing our fundamental knowledge in the development of new alloys. It is also hoped to initiate work in the problems of stress-corrosion cracking.

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

Contract: W-7405-eng-48

Brief Title: THE INFLUENCE OF MICROSTRUCTURE ON THE PHYSICAL PROPERTIES OF MATERIALS

Investigators: J. Washburn

Scope of Work

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 single x-ray scattering, plastic flow stress, ductility and mode fracture with direct observations of defects by means of transmisssion 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 molybdenum and tantalum crystals.

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

Contractor: Cornell University, Ithaca, New York

Contract: AT(30-1)-2504

Brief Title: A STUDY CONCERNED WITH THE BEHAVIOR OF POINT DEFECTS IN SOLIDS WITH EMPHASIS ON THE INFLUENCE OF HYDROSTATIC PRESSURE

Investigators: Arthur L. Ruoff

Scope of Work

Activation volumes and activation energies are being measured for the high temperature creep process in metals. Our work on lead is being extended to near the melting point and similar work will be carried out on aluminum. The pressure range is 1 bar-10 kilobars. Special attention is being given to the creep of the alkali metals. Lithium, sodium and potassium are currently under study and this work will be extended to cover cesium and rubidium. Work has begun on ductile bismuth wire.

Apparatus is designed and will be constructed for the measurement of the energy of vacancy formation in lithium by the cell parameter-dilation method. The double crystal method is to be used to measure change of cell parameter and interferometry is to be used to measure length changes.

Nuclear magnetic resonance effects in aluminum will be studied as a function of pressure. Design work has begun on a device for measuring the effect of pressure on the concentration of quenched-in vacancies and for continuously recording the annealing out of quenched-in vacancies in aluminum. The above studies will help form a comprehensive array of data on the vacancy in aluminum.

Theoretical work is underway in an attempt to explain the creep behavior found. Fundamental research on the basis of reaction kinetics, specifically, vacancy motion has begun. Attempts are being made to discover the validity, as applied to crystals, of the equilibrium assumption in the Eyring theory and the harmonic assumption in the Slater theory.

Contractor: Cornell University (Department of Engineering Physics)
Ithaca, New York

Contract: AT(30-1)-2471

Brief Title: STUDY OF IMPERFECTION IN CRYSTALS BY MEANS OF RELAXATION TYPE MEASUREMENTS

Investigators: H. S. Sack

Scope of Work

The objectives of this research have been to study defects in metallic and ionic materials by internal friction measurements. Bordoni-type internal friction peaks were found in Mo and Nb and investigated as a function of cold work at 2 and 40 kc. The Bordoni peak in Cu was studied in a newly-developed torsion pendulum at 10 cps and a comprehensive evaluation of activation energy and peak width as measured by different authors was made. The influence of impurities on the Bordoni peak also was investigated.

The program for the coming year is essentially a continuation of the present internal friction work with more emphasis on ionic crystals and extension of the experiments to higher temperatures and higher frequencies. Dielectric and conductivity measurements have been started with the objective to study the behavior of point defects (vacancy pairs, electron traps, etc.). Such measurements will be correlated with internal friction measurements, where possible.

Contractor: (The) Franklin Institute Laboratories for Research and Development, Philadelphia, Pennsylvania

Contract: AT(30-1)-2585

Brief Title: STUDY OF THE X-RAY EFFECTS CAUSED BY POINT DEFECTS IN METALS

Investigators: F. R. L. Schoning

Scope of Work

Theories have been proposed which account for the resulting changes of a crystal lattice after the introduction of point defects. It is the aim of this study to correlate the theoretical predictions with experimental results obtained on metal-oxygen and metal-hydrogen systems. For the titanium-oxygen system the lattice parameter and intensity changes are measured as a function of the oxygen concentration. From the lattice parameter the number of interstitial oxygen atoms and the volume expansion are calculated by making use of published data. Knowing concentration and expansion it is possible to predict the intensity changes after adapting the existing diffraction theories to the hexagonal, aeolotropic lattice of titanium. The experimental values of the intensities scattered at the Bragg angles are then compared with the theoretical predictions.

Contractor: IBM Research Center, Yorktown Heights, New York

Contract:

Brief Title: DEFECTS IN METALLIC AND IONIC CRYSTALS

Investigators: Arthur S. Nowick

Scope of Work

This research constitutes a general program of study of the behavior of defects and their effects on metallic and ionic crystals. The research may be considered to fall in the following categories:

A. Work in Metals
   1. Relaxation effects due to point defects created by deformation.
   2. Relaxation effects due to vacancy-solute interaction.
   3. Mechanism of vacancy formation and precipitation in Ag-Zn solid solution.
   4. Comparison between magnetic and anelastic relaxation.
   5. Theory of anelastic relaxation phenomena.

B. Work on Alkali Halides
   1. Comparison of dielectric and anelastic relaxation processes due to vacancy-impurity complexes.
   2. Conductivity and dielectric relaxation in deformed crystals.
   3. Nature of polarization effect above room temperature.
   4. Preparation of ultrapure alkali halides.

Contractor: Illinois, University of, Urbana, Illinois

Contract: AT(11-1)-67, Proj. No. 9

Brief Title: ANNEALING OF COLD WORKED METALS

Investigators: Paul A. Beck

Scope of Work

Information is sought as to the effect of a solute on the mechanical and thermal polygonization of Zn. The arrangement of dislocations in single crystals of high purity Zn and of Zn containing 0.07% Cu has been determined by etching after various bending and annealing treatments. The study is being extended to single crystals of Zn containing 0.04% Al.

A double rolling-texture may be produced in Al, which also produces a two-component recrystallization texture. According to oriented growth theory such a texture should develop only if the recrystallized grains are larger than the deformation bands of the initial two-component structure. An attempt is being made to test the theory by controlling the recrystallized grain size, utilizing the inhibiting effect of a second phase in an Al alloy containing 0.8% Mn and 0.1% Si. A change in the recrystallization texture with grain size could be explained without the assumption of oriented nuclei.

Transmission electron microscopy is to be utilized in studying the structural changes brought about by plastic deformation and subsequent annealing. Two aspects of this work include (1) determination of any correlation which may exist between the formation of recrystallization nuclei and the existing substructure of high purity Al, and (2) the mechanism of annealing out of stacking faults in Cu and its relation to stacking fault energy.

Contractor: Illinois, University of, Urbana, Illinois

Contract: AT(11-1)-833

Brief Title: ELECTRON AND NUCLEAR MAGNETIC RESONANCE

Investigators: Charles P. Slichter

Scope of Work

At present the main activities of this contract are directed towards studying point imperfections in solids by nuclear and electron magnetic resonance. The nuclear resonance studies are primarily concerned with metals, the electron resonance with insulators.

1) Screening of electric fields in metals.

When a point charge is put into an electrical conductor, the electrons readjust themselves to screen out the field of the extra charge. Such an idealized system can be realized by putting an atom such as Al with 3 valence electrons into Cu (one valence electron). Recent theoretical work by Friedel and experimental work by Rowland have shown that earlier ideas about the screening were incorrect. Instead of having a redistribution of charge which dies out exponentially as one goes away from the impurity, the readjustment charge actually oscillates in sign. The readjustment charge produces a change in the Knight shift of nuclei in the vicinity of the impurity, as well as a coupling to the electric quadrupole moment. We are attempting to measure both quantities to obtain more detailed information about the laws of screening.

2) Adiabatic Demagnetization in a Rotating Coordinate System.

Redfield has shown that under certain circumstances, the nuclear resonance in solids is most simply understood by viewing the problem from a reference system rotating at the frequency of the applied alternating fields and applying thermodynamics in this reference frame. A set of "thermodynamic" experiments to test Redfield's idea are being performed. Viewed from the rotating reference frame, they are analagous to ordinary adiabatic demagnetization. The results appear to be very sensitive to electric quadrupole coupling. It is hoped they will lead to a sensitive method of studying point imperfections.

3) Structure of Point Imperfections in Insulators.

By means of electron spin resonance, the structure of point imperfections in insulators - principally alkali halides is being studied. It is possible, by measuring the coupling of the electron to the magnetic moments of nuclei, to determine the electron wave function. Studies of F centers in a number of crystals have been completed. The centers associated with electrons trapped at divalent positive ions (for example, Cd^{H}) present substitutionally for the alkali and centers associated with iron present in silver halides also are being investigated.

Contractor: Little, Arthur D., Inc., Cambridge, Massachusetts

Contract:

Brief Title: ROLE OF LATTICE IMPERFECTIONS IN BEHAVIOR OF SOLIDS

Investigators: Richard S. Davis

Scope of Work

This research on crystalline solids deals primarily with the interactions between imperfections. A secondary phase of the program is concerned with basic oxidation mechanisms.

The research on imperfection interaction stems from earlier work in which the formation of surface pits was observed upon cooling Al from elevated temperature. The pit formation was attributed to vacancy condensation; a one-to-one correlation between the pits and the termini of dislocations at the surface has since been shown. A study now will be performed in greater detail of the factors which cause dislocations to act as either sinks or sources of vacancies. Initial experiments will be performed to determine the effect of various types of low-angle boundaries upon the observed phenomenon. The oxidation research will be based upon a technique which involves forming a surface oxide upon a metal, inducing pit formation, and then stripping the oxide from over the pit with a replica. This technique permits study of the morphology and crystallography of oxide films at various stages of growth.

Contractor: Massachusetts Institute of Technology, Cambridge, Massachusetts

Contract: AT(30-1)-1002, Scope III

Brief Title: IMPERFECTIONS IN METALS

Investigators: B. L. Averbach

Scope of Work

Several x-ray diffraction methods, including line-shape analysis, double-crystal rocking curves, double Bragg scattering at small angles, and measurements of short-range order and atomic displacements, are being used to study the imperfections introduced into metals by plastic deformation, radiation damage, and phase transformations. Etch pit and other metallographic techniques are also being used to investigate features of the dislocation arrays introduced by these various damage processes.

Contractor: Massachusetts Institute of Technology, Cambridge, Massachusetts

Contract: AT(30-1)-1310

Brief Title: MECHANICAL PROPERTIES OF METALS AT LOW TEMPERATURES

Investigators: W. A. Backofen

Scope of Work

Constraint is one of the principal reasons for the difference in deformation behavior of single crystals and polycrystals. Only axial strain is imposed on a single crystal in the tension test, the cross section being permitted to change shape arbitrarily. In contrast, the deformation of each grain in a polycrystal must be compatible with that of its neighbors; as a consequence, lateral as well as tensile strains are imposed. Die-drawing provides an effective way of placing constraints on the single crystals comparable with those in polycrystals; in this way the single-to-polycrystal transition may be bridged more realistically than by use of tensile specimens with only a few grain boundaries (bicrystals, tricrystals, etc.). Preliminary data from such experiments show a marked dependence of both drawing force and lattice rotation on orientation, qualitatively in accord with predictions of the Taylor theory. The finding of single-crystal drawing forces varying with orientation from below to above the polycrystal force is strong support for believing that differences in constraint underlie the usual comparison of single-crystal and polycrystal deformation behavior. An appearance of deformation bands in certain drawn crystals, however, suggests that the Taylor theory is somewhat over simplified. Further work along these lines should lead to a better understanding of both texture formation in polycrystals and the texture-dependence of hardening.

A study of strain hardening in copper single crystals deformed in tension at low temperatures has recently been started. Crystals of orientations $\lfloor 100 \rfloor$, $\lfloor 111 \rfloor$ and $\lfloor 110 \rfloor$ are to be tested at temperatures down to $4.2^{\circ}K$. With these orientations, a number of slip systems are expected to operate simultaneously. Of particular interest will be the effect of interaction of slip systems on hardening characteristics. To date, a horizontal crystal-growing technique has been developed and seed crystals are being prepared.

Another part of the low-temperature mechanical-behavior program is focused on the problem of unstable plastic flow leading to the formation of localized regions of high shear. There is strong evidence of close relationship between unstable flow and shear fracture. Aluminum single crystals with orientation near $[111]$ are being tested, as such crystals reach particularly high flow stresses at low temperature and are prone to exhibit both the unstable flow and shear fracture. Currently, effects of flow stress and work hardening rate are to be studied as orientation around $\lfloor 111 \rfloor$ is varied.

Contractor: Massachusetts Institute of Technology, Cambridge, Mass.

Contract: AT(30-1)-858

Brief Title: X-RAY STUDY OF DEFECTS

Investigators: B. E. Warren

Scope of Work

A new x-ray method has been developed for measuring grain size in the region from 1 micron up. If the primary beam of a diffractometer is narrowed so as to illuminate only a relatively small number of grains, there will be large variations in the measured intensity when the beams falls on different parts of the specimen. From the statistical fluctuations in the relative intensities, an average grain size is given by a very simple equation. By a suitable choice of beam size and slit openings, it is possible to measure independently the size of grains and sub-grains. The method requires very little time, and it can be used on the standard commercial diffractometers. The method has been reported in the J. Appl. Phys. 31, 2237 Dec. 1960, and is now being applied in a large number of laboratories both in this country and abroad.

There is great interest today in the x-ray diffraction study of the structure of molten alloys. These involve more than one kind of atom, and the approximation methods which have been used in the past for interpreting the measurements are not adequate. During the last year a completely general and completely rigorous formulation of the theory and procedure for interpretation has been developed; this formulation will be published soon.

The use of order-disorder as a tool in the x-ray study of the nature of cold work is being applied to the alloy Cu_3Au. There are no results as yet to report.

Contractor: National Bureau of Standards, Washington, D.C.

Contract: NBS Project No. 0901-11-09410

Brief Title: EFFECT OF MICROSTRUCTURE ON THE MECHANICAL PROPERTIES OF CERAMICS

Investigators: F. P. Knudsen

Scope of Work

Many of the mechanical properties of polycrystalline ceramics are notoriously structure sensitive. The objectives of this research project are, (1) to determine which microstructural features govern the structure-sensitivity of the strength of porous brittle polycrystalline bodies, (2) to formulate an expression defining the dependence of strength on these microstructural features, (3) to determine and define the temperature dependence of the relation of strength to these features, (4) to increase the understanding of "why" as well as "how" these microstructural features influence strength.

The project developed a general expression relating the strength (S) of brittle polycrystalline bodies to their porosity (P) and grain-size (G),

$$S = kG^{-a} e^{-bP}$$

wherin k, a, and b are empirical constants which are partially dependent on the test temperature

The expression has proven to be very useful in evaluating the strengths of polycrystalline bodies of dissimilar porosities and grain sizes and in evaluating the effect, on strength, of a change in temperature or changes in composition.

At present the project is investigating the temperature dependence of the strength/porosity/grain-size relationship. In pursuit of the fourth objective, mentioned previously, the project is also investigating, by non-destructive sonic resonance testing, the effect of porosity and grain-size on the elastic and anelastic behavior of brittle polycrystalline bodies between room temperature and approximately 1300°C.

Contractor: Pennsylvania, University of, Philadelphia, Pennsylvania

Contract: AT(30-1)1893

Brief Title: THE EFFECT OF STRESS ON RECOVERY

Investigators: N. Brown

Scope of Work

One objective of this research is to determine the minimum stress at which dislocation movement can be detected in the stress-strain test. The stress at which dislocation movement can be detected in polycrystalline Al depends on the strain sensitivity. By varying the strain sensitivity from 2×10^{-6} to 0.1×10^{-6} it was found that the smallest stress at which dislocations could be detected was 325 psi. This stress was independent of strain (0.8%) and temperature (RT to liquid nitrogen) and varied slightly with impurity content. The minimum stress apparently is related to the resistance of the perfect lattice to dislocation movement.

Dislocation movement could be detected in single crystals at a resolved shear stress of about 60 psi. This value is about 0.3 times the shear stress for polycrystals. Results by other investigators (Averbach and Coworkers) have measured the microyield point of Al and also find that the single crystals yield at about 0.1 the shear stress of a polycrystalline specimen. It was therefore surprising that the grain size exerted no effect on the microyield point or even on the subsequent stress strain behavior.

Although the stress at which dislocation movements was detectable was found to be independent of temperature and strain, the stress to produce a detectable permanent strain (10^{-6}) was greatly strain and temperature dependent. These results indicate that a permanent plastic strain is associated with the intersection and combination of dislocations. The smallest stress at which dislocation movement could be detected was associated with bowing. It appears that the average distance between dislocation nodes is very much greater in single crystals than in polycrystals, and thus bowing is easier to detect.

It is interesting to note the variation of the minimum stress at which dislocations movement can be detected in different crystals. In Zn crystals dislocations can be moved at 1 psi, in Al 60 psi and in polycrystalline Fe 5000 psi. It is believed that these widely different stresses are associated with the basic resistance of the lattice (Peierls-Nabarro Force).

Contractor: Pennsylvania, University of, Philadelphia, Pennsylvania

Contract: AT(30-1)-2151

Brief Title: ORIGIN OF DISLOCATIONS

Investigators: Doris Kuhlmann-Wilsdorf

Scope of Work

The purpose of the investigation is to clarify the behavior of supersaturated thermal vacancies in metals, the way in which they form prismatic dislocations, and how they interact with dislocations. Equipment and techniques have been developed for the preparation of thin single-crystal gold and silver foils gained through electro-deposition from aqueous solutions, as well as for growing thin single crystal wires of aluminum and other metals at ambient temperatures within a few degrees centigrade of their melting points. Into such specimens various concentrations of thermal vacancies may be introduced through suitable heat treatments. They are then to be investigated by means of x-rays, and mechanical and electrical tests. A specialized type of straining apparatus with automatic recording was constructed for the thin foils and single crystal wires.

Interesting experimental results have been obtained on gold foils 1.5 to 30 microns thick. Theoretical research under the present contract contributed to the following two publications: "Considerations on the Interactions Between Thermal Vacancies and Dislocations", by H.G.F. Wilsdorf and D. Kuhlmann-Wilsdorf, Phys. Rev. Letters, 3, pp. 170-172, August 1959 and "On the Behavior of Thermal Vacancies in Pure Aluminum" by D. Kuhlmann-Wilsdorf and H.G.F. Wilsdorf, J. Appl. Phys. 31, pp. 516-525, March 1960.

Contractor: Princeton University, Princeton, New Jersey

Contract: AT(30-1)-2680

Brief Title: LATTICE AND ELECTRONIC DEFECTS IN SOLIDS

Investigators: R. Smoluchowski

Scope of Work

The initial research programme is being developed in three main sections: (1) continuation of ionic conductivity measurements on deformed crystals, (2) thermoluminescence and optical studies of irradiated crystals and (3) crystal growth from solution.

The ionic conductivity measurements are to be made on crystals that have been deformed uniaxially. A suitable press and a furnace have been fabricated. In the field of optical and luminescence measurements the fabrication of the necessary subsidiary equipment, photomultiplier power supply, crystal holders etc. is well underway. A design has been completed for the shielding and mounting of a 150 kv Phillips x-ray apparatus and a Cary recording spectrophotometer is being suitably modified to enable these measurements to be made with maximum facility. Crystal specimens have been produced by crude techniques and these are now being improved.

Silver Halides

Electron trapping in single AgCl crystals is being studied by observing the transient polarization currents in response to a square wave voltage following intense UV illumination. The experimental results agree quite well with a theory based on the build-up and decay of a sheath of trapped holes at the electrodes upon reversal of the applied voltage, assuming no electron injection from the electrodes. These transient currents have been correlated with the thermal release of trapped electrons. From the dynamics of the polarization process one can determine the liberation rate for the trapped electrons and their activation energy.

Contractor: Stanford University, Stanford, California

Contract: AT(04-3)-326, Project No. 2

Brief Title: EFFECT OF LATTICE VACANCIES ON MECHANICAL BEHAVIOR OF CRYSTALLINE MATERIALS

Investigators: Oleg D. Sherby

Scope of Work

Efforts are centered on a study of the kinetics and mechanism of strain softening in metals at elevated temperature. Large strain softening effects have been observed in pure iron in the alpha and gamma phases. Deformations of $\gamma = 300\%$ and over were achieved by torsion tests conducted under constant stress. Typically, the rate of plastic flow, $\dot{\gamma}$, increases over ten times with large deformations and appears to follow the relation $\dot{\gamma} = K\gamma$. This softening effect is probably due to the introduction of lattice vacancies generated by dislocation intersection processes; these excess vacancies increase the self-diffusivity of atoms which in turn accelerate the dislocation climb rate and hence a weaker material results.

Strain softening does not occur until a certain amount of deformation is achieved. This "critical strain" is currently being associated with the condition where the number of vacancies generated mechanically just becomes equal to the number of thermal equilibrium vacancies. In harmony with this consideration, the "critical strain" increases with increasing temperature in both phases of iron. The results obtained permit a direct evaluation of Q_f, the formation energy of a vacancy. Analyses of current results suggest that Q_f equals one half the activation energy for volume self-diffusion Q_d.

Contractor: Union Carbide Nuclear Company, Oak Ridge National Laboratory
Oak Ridge, Tennessee

Contract: W-7405-eng-26

Brief Title: STRUCTURE OF METALS

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

Scope of Work

The purpose of this program is to study the principles dictating atom rearrangements brought about by plastic deformation and thermal treatment.

Studies of plastic deformation include determination of the factors influencing preferred orientation development, the role of stacking faults in deformation processes, and the nature of twinning in the refractory metals. Deformation at high strain rates and studies of ductile fracture may be included.

Annealing processes are being investigated with special reference to effects on preferred orientation. Segregation of solute atoms to stacking faults as a mechanism for hardening is under experimental study.

X-ray studies of atom movements during transformation at low temperature and high pressures will be continued.

Contractor: Union Carbide Nuclear Company, Oak Ridge National Laboratory, Oak Ridge, Tennessee

Contract: W-7405-eng-26

Brief Title: DEFORMATION OF CRYSTALLINE SOLIDS

Investigators: R. O. Williams and J. A. Wheeler

Scope of Work

Topics under current investigation include measurements of the stored energy of deformation in metals and alloys, the kinetics of the release of this energy during recovery and recrystallization, the formation of fiber textures in individual grains during drawing and a study of the early stages of precipitation by means of x-ray diffraction.

Most progress has been made in carrying out measurements of stored energy 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°C and 25°C although runs have so far been made only at -30°C and 25°C.

Contractor: Virginia, University of, Charlottesville, Virginia

Contract: AT(40-1)-2488

Brief Title: THE INFLUENCE OF THE STATE OF THE SURFACE ON THE MECHANICAL PROPERTIES OF CRYSTALLINE MATERIALS

Investigators: J. Mitchell and N. Cabrera

Scope of Work

The purpose of the work is to produce (a) single crystals of metals and alloys with minimum dislocation densities (b) polycrystalline bars and rods of high purity metals and alloys. These materials will be used for the study of the influence of the orientation and state of the surface on the generation of dislocation loops at the surface. We believe that this process is important at the yield point during the earliest stages of plastic deformation.

Apart from the super-electron microscope, the equipment which has been purchased has now been installed and the majority of the basic techniques which will be used during the preliminary exploratory stages of the investigation have been established. Satisfactory methods have been worked out for preparing the surfaces of specimens and for making the points of emergence of dislocations visible by the formation of etch pits. Pre-shadowed carbon replicas of the surfaces have been examined in the Philips 100 B electron microscope. An extensometer has been designed here and constructed in our own workshop. Equipment for preparing and thinning specimens by electrolytic methods has also been designed and constructed. With such thinned specimens, the generation and multiplication of dislocations in metal foils has been directly observed in the electron microscope.

Contractor: Western Reserve University, Cleveland, Ohio

Contract: AT(11-1)-493

Brief Title: POINT IMPERFECTIONS IN METALS

Investigators: Stefan Machlup

Scope of Work

Point imperfections (lattice vacancies and interstitials) have been shown to the important in the process of interdiffusion of metals, as evidenced by the Kirkendall effect; they are thus very likely to be responsible also for self-diffusion. Continued study will be directed to the influence of such defects on the properties of metals and insulators -- resistance, thermoelectric power, specific heat, thermal conductivity.

Interest is at present focused on the distribution of the electronic charge in the vicinity of vacancies and interstitials in alkali metals. The contribution of point scattering of phonons to the thermal resistance of insulators (and some metals) also is being investigated.

Section II-C

Transport Properties of Solids

Contractor: Arizona, University of, Tucson, Arizona

Contract:

Brief 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, which will utilize 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 will involve determination of the activation volume for impurity diffusion and study of the effect of pressure on the screening radius. Initial studies will be 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.

Contractor: Brookhaven National Laboratory, Associated Universities, Inc. Upton, Long Island, New York

Contract: AT(30-2)-Gen-16

Brief Title: DIFFUSION STUDIES IN CERAMIC MATERIALS

Investigators: Alan Auskern and D. H. Gurinsky

Scope of Work

This program is concerned with the determination of the diffusion of gaseous fission products in lightly irradiated uranium carbide powders. Uranium monocarbide is being studied now.

Commercial powders as well as laboratory prepared materials are being investigated. Powders are prepared by the reaction between uranium and methane at about 600 C. Considerable effort is being spent to develop procedures which result in uranium carbide powders of high purity.

The diffusion experiment will consist of a short, low temperature ($50^{\circ}C$) reactor irradiation, followed by a series of out-of-pile high temperature anneals. The gases evolved from the powder at each temperature will be collected on activated charcoal, and the quantities present determined by radioactive counting methods. Proper analysis of the rate of gas release data together with a knowledge of the particle geometry, assuming the release is governed by diffusion, permits the calculation of a diffusion coefficient. Variation of the diffusion coefficient with temperature yields the activation energy for the diffusion process and the frequency factor. The magnitudes of these, and information on uranium and carbon self diffusion in UC can give information on the mechanism of fission gas diffusion.

Contractor: California, University of, Riverside, California

Contract:

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

Investigators: A. W. Lawson and R. L. Wild

Scope of Work

This research is a study of pressure-induced metallic conductivity in transition metal oxides and related compounds. A primary goal will be the investigation by both experimental and theoretical methods of the variation in the electronic band structure of solids as the interatomic distance is altered because of the influence of pressure. The effect of pressures up to 100 kilobars will be examined.

The materials to be studied include the following:

a) rock salt type compounds such as MnO, FeO, NiO, CoO, TiO, VO, and CrN;

b) Corundum structures such as Cr_2O_3, alpha Fe_2O_3, Ti_2O_3, and V_2O_3;

c) Rutile structures such as TcO_2, VO_2, CrO_2;

d) NiAs structures

Contractor: Carnegie Institute of Technology, Pittsburgh, Pennsylvania

Contract: AT(30-1)-2314

Brief Title: SURFACE DIFFUSION ON METALS

Investigators: P. G. Shewmon

Scope of Work

From the rate at which grain boundary grooves form on copper surfaces it is possible to determine the surface diffusion coefficient D_s on the exposed surface. Attempts have been made to apply this technique to various surfaces of silver. Projects started more recently include: (a) The study of D_s at several temperatures, on a variety of surfaces on copper, using the grain boundary grooving technique. (b) A study of the variation of surface free energy of copper with the orientation of the exposed surface. (c) The determination of the grain boundary diffusion coefficient in twist boundaries of silver using a tracer technique (previously published studies have dealt only with tilt boundaries). (d) The determination of the surface diffusion coefficient on gold using a tracer technique. This last project is being done in conjunction with Dr. N. Gjostein of the Ford Scientific Labs. who is doing work on the kinetics of grain boundary grooving on gold bicrystals.

Contractor: Cornell University, Ithaca, New York

Contract: AT(30-1)-2391

Brief Title: THERMAL CONDUCTIVITY OF NONMETALS AND RELATED STUDIES OF TRANSPORT PHENOMENA

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

Scope of Work

During the past year in the theoretical part of this contract, the energy levels of fine particles have been studied, and implications of the discreteness of these levels for the Knight shift and other properties have been examined. During the next year, it is proposed to continue the general study of transport topics (thermal, thermoelectric) in collaboration with the more general study elsewhere in the Cornell theoretical group. Specifically, scattering from imperfections will be analyzed, and associated studies of details of lattice vibration, dislocations of anharmonicity, and structure of defects will be made.

During the past year in the experimental part of the contract two new apparatus for measuring thermal conductivity at low temperatures were designed and largely constructed, and two other apparatus were moved and set up in a more effective way. The scattering of phonons by F-centers at low temperatures was explored thoroughly. This work will be continued with experiments on F- to F'-center conversion at low temperatures. The object of these experiments is to separate core effects from long-range effects in phonon scattering. Measurements on NaCl crystals reveal a striking difference in thermal conductivity of Baden (natural) crystals and Harshaw (melt-grown) crystals, with the Baden crystals better conductors by a factor of 20-50. The possible connection between this observation and the OH^- band in the melt-grown crystals will be investigated. Experiments on the scattering by Mn ions will be undertaken, and the scattering by colloids and dislocations will be studied in appropriate systems. During the past year zone refining equipment was developed for purifying alkali halides, and preliminary experiments were undertaken. These experiments will be continued on NaCl, KCl, and LiF.

Contractor: (The) Franklin Institute Laboratories for Research and Development, Philadelphia, Pennsylvania

Contract: AT(30-1)-2693

Brief Title: STUDY OF THE SURFACE DIFFUSION OF METALS

Investigators: James B. Drew and Henri Amar

Scope of Work

The surface diffusion of metal systems is being investigated through the application of a radio-tracer technique. The diffusion profiles are obtained by autoradiography. In order to make estimates of the activation energy, data have been obtained as a function of temperature. Currently under study are the Ag-Ag, Ni-Ni and Ni-Ag systems.

The question of the possibility of anisotropy lends itself to solutions since a method has been derived which enables diffusion coefficients to be determined as a function of crystalline orientation and direction. The effects of "parasitic" volume diffusion are studied by carrying out the anneals over a wide range of temperatures.

The theoretical phase of this program is concerned with a mathematical solution of the diffusion equation which includes the effects of both volume and surface migration. This leads to two coupled boundary value problems in two and three dimensions, having delicate boundary conditions in the source region.

A critical analysis of previous papers on the formation energy of vacancies and a revised calculation have been performed.

Contractor: Georgia Institute of Technology, Atlanta, Georgia

Contract: AT-(40-1)-2420

Brief Title: MECHANISM AND ACTIVATION ENERGY STUDIES FOR DIFFUSION THROUGH SINGLE CRYSTAL AND POLYCRYSTALLINE HIGH TEMPERATURE MATERIALS

Investigators: Willis E. Moody, Jr.

Scope of Work

This program has as its objective the investigation of inert gas diffusion through non-metallic materials. Initial studies deal with the mechanism of helium diffusion through alumina with single crystals oriented differently and with polycrystalline alumina of various densities. The feasibility of the determination of concentration gradients of A, Kr and Xe by means of x-ray spectrographic techniques will be investigated.

Some time will be devoted to the development and analysis of a high temperature bond between urania and alumina.

Contractor: Illinois, University of, Urbana, Illinois

Contract: AT(11-1)-67, Project No. 3

Brief Title: DIFFUSION IN SOLIDS

Investigators: David Lazarus

Scope of Work

The program is concerned with experimental and theoretical investigation of the nature of defects responsible for diffusion in solids, particularly intermetallic diffusion. The experimental techniques involve precision sectioning methods using radioactive tracers, anelastic relaxation measuremtns, measurements of electrical resistivity, magnetic resonance techniques, and methods for generating high hydrostatic pressures. Diffusion measurements have been performed in the noble metals, copper, silver, and gold, and their binary alloys, both with and without the presence of chemical concentration gradients. Much of the data have been successfully interpreted in terms of a model which considers the electrostatic interactions between a screened impurity atom and solvent atom. Work has been undertaken to investigate the correlation effect by measurement of the mass dependence of diffusion. The effect of pressure on diffusion has been studied in a numer of interstitial and substitutional systems to determine details of the atomic jump process.

Contractor: Maryland, University of, College Park, Maryland

Contract: AT-(40-1)-2068

Brief Title: PROCESSES OF DIFFUSION AND ELECTRICAL CONDUCTION IN SOLIDS

Investigators: Homer W. Schamp, Jr.

Scope of Work

The contractor proposes to accomplish the following objectives:

(1) Continuation of diffusion studies at high pressures and temperatures, particularly of the alkali halides.

(2) Consideration of other experiments which appear to be feasible with the present high-pressure apparatus.

If time permits, studies of the following related phenomena will be conducted:

(a) the mathematical relationship between the diffusion coefficient of the crystal and the melting temperature when the melting point is not a linear function of pressure.

(b) phase transitions of the crystals at elevated pressures.

(c) the electrical conductivity of the alkali halides as a function of pressure and temperature.

Contractor: Massachusetts Institute of Technology, Boston, Mass.

Contract: AT(30-1)-1975

Brief Title: EFFECTS OF STRAIN ON THE DIFFUSION PROCESS

Investigators: B. L. Averbach and Morris Cohen

Scope of Work

The influence of plastic flow on self-and interdiffusion is being studied. The self-diffusion of alpha iron, of nickel, and both the interdiffusion and zinc self-diffusion in aluminum-zinc alloys are being determined as a function of strain, strain rate, temperature, and (in the case of the aluminum-zinc alloys) composition. This work was undertaken in an effort to observe the influence of imperfections on diffusion and also the interrelationship between diffusion and creep.

Contractor: North Carolina, University of, Chapel Hill, N. C.

Contract: AT(40-1)-2036

Brief Title: RESEARCH IN INTERMETALLIC DIFFUSION

Investigators: Lawrence Slifkin

Scope of Work

Studies of self-diffusion in silver-rich alloys of the Ag-Au system have shown that the activation energies for diffusion of both constituents decrease with increasing gold content, even though the melting point is steadily increasing. The pre-exponential factor also decreases with increasing gold content, with that for gold being unexpectedly greater than that for silver. At a given temperature, D for either tracer passes through a shallow minimum; this behavior will be exploited in Kirkendall-tracer experiments in which D will be almost independent of distance through the couple. It is also hoped that the "static" experiments (i.e., no chemical gradients) will be completed all the way across the composition range this year.

It is planned to initiate experiments on self-diffusion in alloys which show order-disorder. The experiments will involve temperature cycling specifically to explore the dynamic effects on the atomic mobility of the approach to equilibrium order. (Such an experiment was suggested some years ago by C. T. Tomizuka.)

Plastic deformation of AgCl crystals has been shown to produce a transient enhanced ionic conductivity attributed to production of excess interstitial silver ions. Large voltage differences are also often observed across the specimen. Both of these studies will be extended to lower temperatures, a variety of types of deformation, and with specimens of various orientations and purity.

Contractor: Pennsylvania, University of, Philadelphia, Pennsylvania

Contract: AT(30-1) 2331

Brief Title: PIPE-DIFFUSION IN SEMICONDUCTORS

Investigators: John N. Hobstetter

Scope of Work

1. During the first year of this contract, four large crystals of n-type germanium having 100 dislocations/cm^2 were prepared. A goniometer jig for wafering these crystals with a diamond saw was built and the crystals were cut into bars oriented critically for single slip in bending. A device for producing controlled bending at high temperatures with 4-point loading were also built and tested. A spring-loaded electrical probe mounted on a stereomicroscope was built and is used to map the diffusion-penetration profile along the germanium specimens. Finally, a jig for grinding tapered sections at accurately known angles was built and tested. The penetration profiles are to be determined on such sections. Several diffusion runs have been made on control specimens.

2. During the coming year, indium will be diffused into germanium bars containing parallel arrays of dislocations of controlled density formed by bending and polygonization. The diffusion anisotropy introduced by these arrays will be studied and attempts made to calculate the pipe effect in this system.

Contractor: Pennsylvania, University of, Philadelphia, Pennsylvania

Contract: AT(30-1)-1879

Brief Title: EFFECT OF STRESSES ON SELF-DIFFUSION OF SILVER SINGLE CRYSTALS

Investigators: R. Maddin

Scope of Work

It has been known that dislocation lines climb at high temperature either by giving off lattice vacancies or by absorbing them. The concentration of vacancies in equilibrium with an edge dislocation, according to the calculation of Bardeen and Herring* will be either

$$N_o \exp (Fb/kT)$$

or $$N_o \exp (-Fb/kT)$$

where N_o is the equilibrium concentration of vacancies with the dislocation in an unstrained lattice, F is the force per atomic length of dislocation line exerted normal to the slip plane, b is Burger's vector, k is Boltzman's constant and T is the absolute temperature. Which of the two equations is valid depends on whether the force F is tending to push the dislocation line in a direction which creates vacancies or annihilates them. However the probabilities of the dislocations existing in two directions are the same. The average vacancy concentration throughout such a crystal therefore will be proportional to:

$$1/2 \; N_o \left[\exp (Fb/kT) + \exp (-Fb/kT)\right]$$

According to this relation, when the applied stress is large enough, it will give an overall excess concentration and hence an enhanced diffusion rate. The magnitude of applied stress seems to be a very important factor in determining the enhanced diffusion rate.

Devices have been designed for applying constant torsional stress to the specimen during diffusion annealing. The primary runs of experiments at 800°C show a positive result. In order to make a complete analysis of stress effect on diffusion, extended work is being performed.

*J. Bardeen and C. Herring, Imperfections in Nearly Perfect Crystals, John Wiley and Son, New York (1952)

Contractor: Rensselaer Polytechnic Institute, Troy, New York

Contract: AT(30-1)-1044

Brief Title: ANISOTROPIC SELF-DIFFUSION IN METALS

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 effect is anisotropic. In the past we have investigated self-diffusion in zinc, cadmium, thalium and indium. About a year ago a start was made to study the diffusion of substitutional impurities in zinc as a function of valence and ion size. The initial results have shown that the diffusion of silver in zinc goes at a rate roughly 1/10 as rapid as the self-diffusion of zinc, while on the other hand the diffusion of indium in zinc is faster by roughly a factor of 10 than the self-diffusion. Moreover the sign of the anisotropy is reversed in the case of the diffusion of indium - this means that diffusion in the basal plane is faster than perpendicular to it. Studies of the diffusion of radioantimony in zinc are at present underway and considerably more work is planned.

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 nickel. The experiments are performed with the marker motion confined to the central portions of the wires as the ends are force cooled. In the case of gold it was found that the mass transport was in the direction of the anode, presumably the result of momentum transfer from the streaming electrons. However, in the case of copper the transport was in the direction of the anode only at low temperatures and reversed itself above 1000°C. Our investigation in platinum indicated that its behavior in general is similar to that of the copper. Future plans call for investigating a wide number of pure metals, several with lower melting points. To determine temperature accurately without pyrometry will require that the specimens be large enough to contain a thermocouple inside them. The larger specimens necessitate a heavy duty DC supply which is just now being completed. The theoretical significance of these phenomena also is under study.

Contractor: Stanford University, Stanford, California

Contract: AT(04-3)-298

Brief Title: KINETICS IN SOLID STATE SYSTEMS

Investigators: Robert A. Huggins, Victor G. Macres

Scope of Work

An active research effort is being carried out on three aspects of solid state kinetics including diffusion in ternary systems, effect of concurrent plastic strain on diffusion, and diffusion in ordered structures at very high temperatures. In these studies, diffusion gradients are being analysed by electron microprobe analysis. The latter aspect of the program will also use nuclear magnetic resonance techniques and radioactive tracers.

In the ternary diffusion program, an attempt is being made to interrelate diffusion and thermodynamic properties in an effort to provide a more basic understanding of the driving force for diffusion. It is expected that this study will provide additional insight on the mechanisms of diffusion and the Kirkendall effect. Studies are being carried out on the copper rich solid solution (alpha phase) of the copper-cadmium-zinc system.

The objective of the program on the effect of concurrent plastic deformation an diffusion is to explore further the role of crystal imperfections in the diffusion process in substitutional solid solutions. Attention is being directed to chemical diffusion (rather than self-diffusion) in systems which exhibit a Kirkendall effect. Specifically, the copper-zinc system is being studied and the investigation is being carried out by comparing diffusion kinetics during the dezincification of beta brass and the zincification of copper with and without concurrent plastic strain.

The purpose of the program on diffusion in ordered structures is to obtain a more basic understanding of the mechanism and kinetics of the diffusion process in such structures. The diffusion of titanium and zirconium cations in single crystals of aluminum oxide as well as diffusion in three-five and four-six semiconducting compounds is being studied.

Contractor: Union Carbide Nuclear Company, Oak Ridge National Laboratory
Oak Ridge, Tennessee

Contract: W-7405-eng-26

Brief Title: CERAMICS RESEARCH

Investigators: D. L. McElroy and C. S. Morgan

Scope of Work:

Scope I. Thermal Conductivity

The thermal conductivity of ceramics such as UO_2, BeO, ThO_2 and UC will be studied and the influence of such factors as grain size, porosity, defects, impurities, and irradiation will be determined. The past emphasis has been the development of suitable equipment to measure both thermal conductivity and thermal diffusivity to cover the temperature range from room temperature to 2700°C. An evaluation of the various techniques is being made.

Scope II. Sintering of Oxides

Present work is directed toward a study of the mechanism of sintering in ThO_2. Experiments include rate measurements both of free compacts and during hot pressing, measurement of rate of diffusion of oxygen and thorium in ThO_2, and studies of the microstructure and surface properties of the starting powders.

Contractor: Wake Forest College, Winston-Salem, N. C.

Contract: AT-(40-1)-2413

Brief Title: A STUDY OF ATOMIC MOVEMENTS IN SOLIDS EMPLOYING ANELASTIC MEASUREMENTS

Investigators: Thomas J. Turner

Scope of Work

Employing an inverted torsion pendulum and an elastic-after-effect apparatus Zener relaxation (stress induced ordering) has been observed in the AgAu system even though there is a negligible size difference. For 58.5% Au in Ag, H= 43.6 + 0.4 $\frac{\text{Kcal}}{\text{mole}}$. In contradistinction to work in other systems this value lies between the value for Ag and for Au into the solid solution. The range of measurements will be extended because better resolution now can be achieved by working with single crystals. This will be done for comparison with the extensive diffusion data being obtained by Professor Lawrence Slifkin.

The effect has been studied in 38.5% AgCd and 20% AgIn yielding H = 34.8 + 0.2 and 34.0 + 0.2 $\frac{\text{Kcal}}{\text{mole}}$ respectively. Ordering peaks were observed in solutions of maximum concentration of AgSn and AgSb. However, now that single crystals can be prepared activation energies for these systems will be obtained. The present work will be extended to high frequencies (25 KC) employing a resonant bar driven electrostatically in an effort to detect any temperature dependence in the activation energy. It is hoped that by examining the effect in a series of solution of Ag and the elements following it in the periodic table, one can determine the mechanism involved.

Section II-D

General Solid State Physics and Physical Metallurgy

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

Contract: W-7405-eng-82

Brief Title: EXPERIMENTS RELATED TO SOLID STATE THEORY

Investigators: R. G. Barnes, R. H. Good, A. V. Gold, D. E. Hudson, J. M. Keller, S. Legvold, D. W. Lynch, and A. R. Mackintosh

Scope of Work

A great part of the current interest in this field lies in a study of the thermodynamic properties of solids. A combination of several types of measurement (elastic constant, magnetic susceptibility, thermal expansion, crystal structure) has been used to attempt to understand the bonding in intermetallic compounds. Measurements of the thermal expansion of anisotropic substances are being carried out over a range of temperatures, and an attempt is being made to obtain thermal expansion data at liquid helium temperatures. The problem of the contribution to the thermal expansion of anharmonicity in interatomic forces has been studied theoretically. Heat capacity measurements (Tb metal, solid He^3 under pressure) have been made down to $0.25^{\circ}K$ in an attempt to understand the nuclear contributions to the thermodynamic properties. The equation of state of the simpler substances is being studied both theoretically (condensed gases, He^3 under pressure) and experimentally to 20,000 atmospheres over a wide range of temperature ($20^{\circ}K$ to the melting point, for the solidified rare gases, alkali metals).

In addition, dilute alloys are being investigated as to the possibility of their use in adiabatic demagnetization experiments. Additional magnetic work includes magnetostriction in ferro- and antiferromagnetic substances, and routine susceptibility measurements on pure single crystals of metals.

Nuclear magnetic resonance techniques are being used to investigate the Knight shift in various intermetallic compounds, and the effect of deformation on the Knight shift in Li, as well as the effect of the ferro- and antiferromagnetic states on the resonances in various iron group halides. The effects of pressure and temperature on the resonances in Li and Na are being used to study self-diffusion in these metals. Diffusion also is being studied (in a different temperature range) using recently adapted mass-spectrometric techniques. Impurity effects in single crystals are being investigated using electron spin resonance methods.

Work on the electronic properties of metals is expanding considerably, with de Haas-van Alphen, ultrasonic attenuation, and magnetorestivity measurements being undertaken on pure metals. Theoretical work in this field also is being done. The thermodynamic properties of superconductors are being obtained from measurements of critical fields as a function of temperature and pressure, with the major emphasis being on the transition elements. This work is being extended to include superconducting compounds.

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

Contract: W-7405-eng-82

Brief Title: THERMOELECTRICITY, SEMICONDUCTORS, INSULATORS

Investigators: G. C. Danielson, J. F. Smith, C. A. Swenson, A. V. Gold, and A. R. Mackintosh

Scope of Work

Most of the work done in this area has been concerned with the properties of the semiconductors, Mg_2Si and Mg_2Ge. The resistivities and Hall coefficients of both of these have been measured for various impurities over a wide range of temperature ($4^{\circ}K$ to $1000^{\circ}K$), and the Seebeck coefficient of Mg_2Si has been measured recently over the same temperature interval, with a definite phonon-drag contribution found at low temperatures. A rather complete study of the other properties of these semiconductors is being undertaken, with a determination of the magnetoresistivity tensor as a function of temperature being completed. Measurements of the elastic constants and optical absorption are in progress, while plans are being made for high temperature measurements of the thermal diffusivity. Measurements of the Hall mobility of germanium at microwave frequencies also have been made. A separate program involves the determination of the thermoelectric power of single crystals of the hexagonal metals.

The sodium-tungsten-bronzes (Na_xWO_3) are being studied as a function of sodium concentration (x) both experimentally and theoretically, in an attempt to understand their properties. This work includes the electrical properties, crystal structure, Knight shift, and the reflection spectra.

A considerable amount of work has been done on diamond, with an optical measurement of the excitation energies of the charge carriers being completed. Results have been obtained using a new method of determining the bulk resistivity of diamond. The optical properties of V centers in the alkali halides also are being studied.

Contractor: Argonne National Laboratory, Argonne, Illinois

Contract: W-31-109-eng-38

Brief Title: SOLID STATE THEORY

Investigators: T. Arai, F. Bassani, F. Fumi, T. Gilbert, A. Rahman, J. Robinson, A. Sjölander, K. Singwi, and M. Tosi

Scope of Work

The solid state theory program has as its general objective the development and application of new theoretical techniques and concepts and the application of existing methods and concepts to give a better understanding of 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 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:

Exchange Interaction and Heisenberg Spin Hamiltonian (T. Arai). The validity of the Heisenberg Spin Hamiltonian for exchange interactions has been confirmed. The Heisenberg Spin Hamiltonian has been derived rigorously as the dominant term in the effective Hamiltonian, settling an existing controversy. The rigorous expression for the exchange forces is being applied to study super exchange forces in antiferromagnets.

Electronic Energy Band Calculations (F. Bassani). A perturbation approach has been developed to calculate the electronic energy levels of solids and has been applied to the diamond structure and to the zinc blende structure. Results have been obtained for silicon and diamond and, using a slightly modified approach, for solid argon. General O.P.W. calculations on BN and on other group III-IV semiconductors will be carried through. The variation of the energy bands with pressure will also be calculated.

Equation of State, Polymorphic Transitions, Ionic Radii and Cohesive Properties (F. Fumi and M. Tosi). The parameters which enter the generalized Mie-Grüneisen equations for the first and second volume derivatives of the lattice energy of a solid have been computed from thermodynamic data. It has been shown that the resulting equations have a wider temperature range of validity than those traditionally used in the Born theory of ionic solids or those adopted more recently by Born and Huang. A theoretical study is underway dealing with pressure transitions of the potassium and rubidium halides. It has been shown that the Born model, somewhat generalized, can account for the transition. A derivation of a new set of crystal radii for the alkali and halogen ions in the alkali halides using the Huggins-Mayer formulation is being completed. The preparation of a review article on the Born theory of the cohesive properties of ionic solids will be undertaken soon.

Ab initio Calculation of Elecronic Structures and Theoretical Studies of Molecule-Ion Centers (T. L. Gilbert). Atomic Hartree-Fock orbitals and energies for F, F, Ne, Na, and Na+ have been calculated Orbitals for F_2 and possibly Cl_2 will be calculated. The application of Hartree-Fock methods to solids is under detailed study. Theoretical studies directed towards giving a detailed interpretation of the optical absorption, thermal decay and paramagnetic resonance line width of the Cl_2 center in a series of host lattices is underway. A one-dimensional model of a Cl_2 center looks very promising. Future work will entail studies of a two-dimensional model. The impurity induced coupling between energy bands is also under study.

Slow Neutron Scattering (A. Rahman, K. Singwi and A. Sjölander). Theoretical studies of slow neutron scattering with direct application to experimental results from Brookhaven and Chalk River indicate the validity of a quasi-crystalline model for liquid water. Such results are not only of basic interest but also of importance in practical neutron thermalization problems. Similar work on lead has led to a damped phonon model which gives very encouraging results. A theory of the Mössbauer effect has also been developed from a space-time-self correlation function point of view. This theory suggests applications of the Mössbauer effect for the study of diffusive motions in solids near the melting point. Work continues toward better standing of liquid structure and dynamics as well as the dynamics of atom motions in solids.

Interference Effects in Electron Scattering from Defect Pairs (J. Robinson). The contribution to the scattering of quasi-free electrons of those interference effects due to the proximity and correlated position of an associated pair of defects is being calculated.

Contractor: Argonne National Laboratory, Argonne, Illinois

Contract: W-31-109-eng-38

Brief Title: ELECTRON AND NUCLEAR MAGNETIC RESONANCE STUDIES

Investigators: E. Avery, D. Connor, J. McMillan, D. O'Reilly, B. Smaller, T. Tsang, and E. Yasaitis

Scope of Work

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.

Electron Spin Resonance (B. Smaller, E. Avery, J. McMillan and E. Yasaitis). Using a variety of operating frequencies and techniques, electron spin resonance and double resonance have been applied to the study of paramagnetic centers of both intrinsic and radiation damage type. Studies continue on the identification and characterization of color centers and impurity centers in alkali halides and of free radicals produced in organic solids and biological systems by irradiation. Studies are also underway on the magnetic properties and electronic structure of rare earth and transuranium salts. Detailed studies of the radiation chemistry of ice and of the radiation decomposition of inorganic nitrates have been completed. Electron spin saturation techniques are under development to obtain nuclear polarization of sufficient magnitude to be useful for the study of nuclear decay processes and especially the inter-relations of the nuclear and solid state aspects.

Nuclear Magnetic Resonance of Short-Lived Nuclides (D. Connor and T. Tsang). A novel nuclear magnetic resonance technique has been developed and has made possible the observation of the nuclear magnetic resonance of several short-lived nuclides by means of the asymmetry in beta-decay from polarized nuclei. The necessary large nuclear polarization is obtained by producing the unstable nuclei by the capture of polarized neutrons. The magnetic moments of many short-lived nuclides can be determined and the depolarization effects due to the solid state environment are admirably studied by this technique. A detailed experiment has been completed on the gyromagnetic ratio of the Li^{8} nucleus. The influence of the solid state environment on the retention of the magnetic polarization is under study both for radiation damaged and undamaged crystalline material.

Nuclear Magnetic Resonance of Stable or Long-Lived Nuclides (D. O'Reilly). The intensities, Knight shifts, and relaxation times of Li^{7} and Na^{23} will be measured for solutions of Li and Na in liquid ammonia at temperatures below 25°C. These data are expected to yield important information on the interaction of electrons and metal ions in metal-ammonia solutions. The

planned measurement of the O^{17} nuclear magnetic resonance in metal oxides enriched with O^{17} will be carried out if proper samples can be obtained. The objective is to determine the electric field gradients in diamagnetic oxides such as Al_2O_3 and electron density information on antiferromagnetic oxides such as Cr_2O_3 and paramagnetic oxides such as the tungsten bronzes.

Contractor: Argonne National Laboratory, Lemont, Illinois

Contract: W31-109-eng-38

Brief Title: PHYSICAL METALLURGY STUDIES OF URANIUM, PLUTONIUM, AND ZIRCONIUM

Investigators: A. F. Berndt, M. B. Brodsky, E. S. Fisher, L. Ianniello, L. T. Lloyd, C. J. Renken, S. J. Rothman, D. G. Westlake

Scope of Work

The over-all objectives of the physical metallurgy studies of the reactor materials are to provide basic data on their structures and properties, and to take advantage of their special structural properties in furthering our knowledge of certain problems in metal physics in general. The scope of the program as evidenced by some of the problems currently under investigation is outlined below.

Elastic Constants of Alpha-Uranium

The nine fundamental elastic moduli of alpha-uranium are being determined by measurement of ultrasonic wave velocities in single crystals. Data are complete for the temperature range between 78° and 310°K. Recent measurements at temperatures below 78°K indicate a transformation at approximately 42°K. Similar effects have been noted at about the same temperature in curves of Hall-coefficient and thermoelectric power as functions of temperatures; whereas, specific heat and lattice parameter data do not indicate a transformation. Upon completion of the low temperature measurements, the studies are to be extended to the alpha to beta transformation temperature. Recent development of a coupling media for affixing the crystal to the transducer will permit measurements of even shear wave velocities up to this temperature.

Thermal Expansion of Alpha-Uranium

Dilatometric measurements of thermal expansion in the three principal crystallographic directions of alpha-uranium have been obtained from single crystals between room temperature and 600°C. Discrepancies between the expansions of single crystals and the expansions calculated from lattice parameter data are believed to be related to the elastic interaction between grains of the polycrystalline samples used for the latter measurements. These studies are being continued to check the lattice parameter data below room temperature and to provide data for the dimensional change of single crystals with temperature.

Plastic Deformation of Alpha-Uranium

Studies of the operative plastic deformation mechanisms in alpha-uranium at room temperature and 600°C have been completed. Twinning and slip in the (010) - [100] systems are important deformations at room temperature; whereas,

at 600°C the predominant slip system is (100) - [100] and twinning is relatively unimportant. This work is being extended to a study of the operative deformations at subroom temperatures, and in investigation of the change in critical resolved shear stresses of the various slip systems as a function of temperatures, both above and below room temperature.

Diffusion in Uranium

The self-diffusion parameters in the gamma and beta phases of uranium have been studied by isotope tracer techniques. The activation energy for self-diffusion in gamma-uranium is anomalously low and the D_o value is high when compared with the values predicted by theories of diffusion by the vacancy mechanism. Further experiments are being performed with the goals of delineating the mechanism of self-diffusion in the gamma phase and of explaining the differences between experimental and theoretical values. Also, experiments are in progress to measure the self-diffusion parameters in alpha-uranium as functions of the crystallographic directions.

A program has been initiated to measure the diffusion parameters of tracer amounts of other elements in the body-centered-cubic gamma-uranium structure. Results are available for diffusion of gold and chromium. This work is to be continued with the aim of correlating the diffusion parameters with solute atom size and valence.

Preparation of High-Purity Plutonium

Techniques have been developed for preparing high-purity plutonium by electrolysis of impure anodes in a fused salt electrolyte. This equipment is being scaled-up so that adequate quantities of high-purity plutonium can be made to support the plutonium research programs.

Properties of Delta-Stabilized Plutonium Alloys

The peculiar negative coefficient of the face-centered-cubic delta phase of plutonium has focused attention on the nature of the electronic structure of this phase. Two approaches to this problem are being investigated. One program deals with the effects of temperature, pressure and composition on electron transport phenomena, such as electrical resistivity and thermoelectric power, in the region of structure transformation. The second approach is a study of the electronic structure of delta-plutonium stabilized with various amounts of other elements by measuring thermal expansion, Hall-coefficients and thermoelectric power as functions of temperature and composition.

Substitutional Solid Solutions of Plutonium in Uranium

As part of an over-all program dealing with the structural features substitutional solid solutions in metals, a study is being made of the lattice parameters of solid solutions of plutonium in alpha-uranium as functions of temperature and composition. The goals of this work are to provide information about both the solute and solvent metal structures. Ultimately this study will be extended to the investigation of other properties and other alloy systems.

Elastic Moduli of Zirconium Single Crystals

As part of a general interest in the behavior of the elastic moduli of transition metals, the ultrasonic wave velocities in alpha-zirconium single crystals are being measured as functions of temperature. Data have been obtained for the five fundamental moduli at room temperature, and measurements are in progress to determine the moduli up to the alpha to beta phase transformation. Also the moduli will be determined down to liquid helium temperatures. The immediate goal of this study is to ascertain if zirconium exhibits deviations of the elastic moduli from normal behavior as does palladium, yttrium and uranium. From a long range viewpoint, the work will be continued to determine if the deviations of the elastic moduli in transition metals obeys some selection rule based on the free atom electron configurations.

Plastic Deformation of Alpha-Zirconium Crystals

As part of an over-all study dealing with solutions of interstitial atoms in a metal, the effects of hydrogen addition to single crystals of alpha-zirconium upon the deformation mechanism are being investigated. A redetermination of the habit planes of zirconium hydride in alpha-zirconium has shown that, for the most part, the hydrides are parallel to the {10.0} planes (the slip planes); some hydrides parallel to {10.5} planes were observed in a sample containing 60 parts per million by weight hydrogen, and a sample containing 175 ppm hydrogen had a few hydrides parallel to {10.1} planes. The goal of the program is to determine the effects of hydrogen content and temperature upon slip and twinning deformations at subroom temperatures and to explain the observed effects in terms of dislocation theory.

Recyrstallization Textures of Deformed Single Crystals of Alpha-Zirconium

In a study of orientation relationships between recrystallized grains, which were created by annealing deformed single crystals of alpha-uranium and the original crystal orientation, it was found that a singular relationship existed between the two lattices provided the grains were assumed to originate from deformation twins as well as from the parent crystal. To determine if this general rule applies to all metals exhibiting deformation by twinning, a similar study of deformed single crystals of alpha-zirconium is in progress. Suitably oriented samples have been prepared and deformed by slip alone or slip plus twinning on {10.2}, {11.1} and for {11.2} planes. The orientations of grains developed by annealing have been determined, and preliminary treatments of the data indicate that a singular relationship also prevails for this metal if the grains are considered to originate from twin orientations as well as from the parent crystal.

Contractor: Argonne National Laboratory, Argonne, Illinois

Contract: W-31-109-eng-38

Brief Title: INELASTIC SCATTERING OF SUBTHERMAL NEUTRONS

Investigators: D. Connor

Scope of Work

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 atomic in crystals. Such studies will complement the theoretical studies already underway.

The experimental program designed to make these studies will get underway first using the conventional techniques of cold beryllium neutron filtering coupled with the use of fast choppers of advanced design. Experimentation with some theoretically simple solids and improvement of the neutron detection system will proceed simultaneously. Since it is essential for advanced experimentation to have the maximum flux of cold neutrons, the development of cryogenic facilities for relatively large scale moderation of reactor neutrons in the useful long wavelength region will be pursued vigorously.

Contractor: Argonne National Laboratory, Argonne, Illinois

Contract: W-31-109-eng-38

Brief Title: PHYSICS OF METALS

Investigators: L. Guttman and J. Mullen

Scope of Work

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

X-Ray Diffraction Studies (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.

Diffusion Studies and Mössbauer Effect Studies (J. Mullen). This program consists in the theoretical study of the effects of correlation on anisotropic diffusion. An experimental program is planned to undertake the measurement of the temperature dependence of anisotropy in diffusion, since such data will be very useful in determining mechanisms of diffusion. Mössbauer experiments are also underway to investigate thermal and magnetic properties of solids and possibly also the diffusive properties near the melting point.

Contractor: Argonne National Laboratory, Argonne, Illinois

Contract: W-31-109-eng-38

Brief Title: LOW TEMPERATURE PHYSICS

Investigators: O. V. Lounasmaa and R. Guenther

Scope of Work

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

The thermodynamic behavior of liquid helium-4 is anomalous in the temperature region near the transition from the normal to the superfluid state. This anomalous behavior is extremely interesting both from the experimental and theoretical points of view. Recent more accurate low temperature experimental data on the specific heat at constant volume and on the pressure coefficient at constant volume, measured as a function of temperature and density, have made it possible to calculate and tabulate the most important thermodynamic functions of helium-4 to an accuracy of 1-2% in the temperature range from 1.5 to 300^{o}K and up to pressures of about 100 atmospheres.

To obtain still greater insight regarding the anomalous behavior of helium-4 very near the λ-curve (normal to superfluid transition curve), apparatus has been constructed to make measurements of the equation of state of liquid helium at temperature intervals of the order of 10^{-5o}K. The fine details of the behavior of liquid helium are exceedingly important for the further development of the theory of liquid helium, and the new measurements underway are expected to be very informative.

The helium-3 cryostat has been completed and tested down to 0.3^{o}K. The related calorimetric equipment for the precision measurements of specific heats has also been assembled and tested. An extensive series of accurate measurements of the specific heats of the rare earth metals will be carried out. These metals exhibit magnetic anomalies at liquid helium temperature and the Debye temperatures are low. No specific heat measurements below 1.5^{o}K have been reported (except for samarium), and it has not been possible up till now to separate lattice and electronic specific heats.

Contractor: Argonne National Laboratory, Argonne, Illinois

Contract: W-31-109-eng-38

Brief Title: OPTICAL AND SPIN RESONANCE PROPERTIES OF SINGLE CRYSTALS - COLOR CENTER RESEARCH

Investigators: P. H. Yuster, C. J. Delbecq, S. Susman, and A. Ghosh

Scope of Work

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:

Investigation of the nature of the self-trapped hole centers, Cl_2, and of the Ag^0 center in silver doped KCl and characterization and study of the more complex $AgCl_4^=$ centers resulting from hole migration and retrapping. The system KBr-KCl will also be studied with respect to hole trapping. Such a system could form Cl_2^-, Br_2^-, and possibly ClBr. The variation in the position and nature of the absorption bands and spin resonance properties as well as the variation in thermal stability properties of the various holes in the same host lattice will be a powerful tool for the further understanding of the electron energy level properties of these defects in relation to the valence and conduction bands of the perfect lattice.

The study of the luminescence emission mechanism in KCl-Tl and especially the role of hole trapping therein. The present day model is oversimplified due to neglect of hole trapping. Also, optical and thermal bleaching data do not agree with model.

Detection and characterization of the spin resonance centers obtained in KCl-KNO_3 upon irradiation. Correlation with other radiation chemical effects.

Preparation of pure KCN (alkali Halide structure) and study of the nature of the optical and spin resonance centers by means of optical and thermal bleaching and photoconductivity measurements.

Contractor: Armour Research Foundation, Chicago, Illinois

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

Brief Title: MAGNETIC PROPERTIES OF INSULATORS

Investigators: J. J. Markham

Scope of Work

The purpose of this program is to understand the magnetic properties of F-centers in a quantitative manner. The F-center in alkali halides shows an interesting paramagnetic resonance signal. The absorption signal is broadened by hyperfine interactions between the electron trapped at the 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. Precise measurements of the spin lattice-relaxation and the coupling between the spins are possible. This will be done on additively colored F-centers in KCl and RbCl. Attempts will be made to obtain a semi-quantitative theory which will amplify our understanding of the interactions between trapped electrons and the surrounding ions which are vibrating. This program will necessitate some optical work on the F-centers so that one may know the properties of the centers on which electron spin measurements are made.

Contractor: Brown University, Providence, Rhode Island

Contract: AT(30-1)-2394

Brief Title: ANALYSIS OF STRUCTURES OF TWO-PHASE ALLOYS

Investigators: J. Gurland

Scope of Work

Research performed to date in this program has dealt with the following subjects:

1. Spatial distribution of discrete particles: This part of the work was concerned with the definition and measurement of topological variables related to the distribution of particles of one phase in multiphase alloys.

   The following concepts were defined mathematically and operationally:

   (a) Degree of dispersion, as related to surface of separation, fineness, and spatial distribution.

   (b) Average distance between particles, namely mean free path and distance between nearest neighbors.

   (c) Condition of particle contact and relation of particle contact to continuity of phase distribution.

2. Statistical description of distribution of phases: An attempt has been made to apply the theory of runs of mathematical statistics to the quantitative description of the state of distribution of phases. Three states of distributions are distinguished: segregated, random and dispersed. A statistical parameter was defined to indicate the degree of segregation or dispersion.

3. Statistics of fracture modes: The work was concerned with the statistical treatment of two modes of fracture: 1) by propagation of a crack from the weakest volume element in the absence of a propagation barrier and 2) by independent, simultaneous or consecutive cracking of individual volume elements separated by a propagation barrier.

During the coming year, it is proposed to continue the statistical analysis of two-phase mixtures with particular reference to the development of a "continuity parameter". For instance, the probability of an infinitely long chain of connected particles could be regarded as such a parameter. The theoretical study will be supplemented by experimental measurements of distribution and continuity of actual and synthetic alloys or mixtures.

In addition, the analysis of the statistics of fracture modes will be extended by a calculation of the strength ratios to be expected from failures by various modes. This study still contains many unsolved problems, many of which must be discussed before a clear understanding is reached.

Contractor: California Institute of Technology, Pasadena, California

Contract: AT(04-3)-221

Brief Title: FUNDAMENTAL STUDIES OF MATERIALS PERTAINING TO NUCLEAR ENGINEERING

Investigators: Pol Duwez

Scope of Work

The study of alloys very rapidly cooled from the melt has produced many new structures in various alloy systems. In gold-silicon alloys, the amorphous phase discovered around 25 atomic percent germanium seems to exist only within a narrow range of compositions. With increasing silicon content, the alloys are crystalline but the powder diffraction patterns are so complex that the structure of the phase or phases present have not yet been established. In addition, many different phases seem to exist depending on the silicon content. Similar results have been obtained in silver-silicon and gold-germanium alloys.

The rapid cooling technique has been modified so that alloys can be quenched to liquid nitrogen temperature and x-ray diffraction studies are also carried out at that temperature. This capability extends the field of investigation to alloys containing metals of relatively low melting points. Without being kept at a low temperature, these alloys would revert to the stable equilibrium phases at room temperature. The most important results obtained so far is the existence of an extended solid solution in cadmium-zinc alloys. In this system, the theory of alloys would predict solid solubility, but under equilibrium conditions a eutectic type phase diagram is found. A detailed study of this system, now underway, will certainly bring out interesting fundamental information on the alloying behavior of metals.

Another interesting feature of rapidly cooled metals and alloys is their extremely small grain size. Electron microscopy (by transmission) of a rapidly cooled foil of copper has shown that the grain size is less than half a micron, and the grains appear to be equiaxed without preferred orientation. This grain size is several orders of magnitude smaller than what has been previously observed in any metal after solidification from the melt. The rapid cooling technique is a new tool for the study of the effect of grain size on the physical properties of metals and alloys.

Contractor: California, University of, Berkeley, California

Contract: AT(11-1)-34, Proj. #47

Brief Title: MICROWAVE FARADAY ROTATION

Investigators: A. M. Portis

Scope of Work

The work being done under this project agreement is directed toward an understanding of the magnetic and electrical properties of solids and particularly metals. A great deal of attention currently is being given to ferromagnetic metals and to the use of nuclear resonance in the study of these metals. Nuclear resonance studies of both alloys and intermetallic compounds are being carried out in an effort to elucidate the role of conduction electrons in ferromagnetism. The ferromagnetic rare earth metals show a complex and interesting behavior. Studies of the microwave ferromagnetic resonance of these metals with single crystals made available by the Institute for Atomic Research are in progress. A second very important area in the physics of metals is that of superconductivity. An experiment designed to detect a microwave Hall effect in superconducting metals is in progress. It is hoped that this technique will permit a detailed study of the transport properties of superconducting metals. One of the most interesting and puzzling of magnetic problems is that of antiferromagnetism. Studies of the antiferromagnetism of ionic solids are in progress. The results of these studies may later be applied to metals.

Contractor: Case Institute of Technology, Cleveland, Ohio

Contract: AT(11-1)-623

Brief Title: SOLID STATE PHYSICS

Investigators: C. S. Smith

Scope of Work

The work which has been done and which is proposed is directed to the experimental study of thin film physics and the elastic constants of crystals and to the theoretical study of the band structure, lattice vibrations and relaxation phenomena in solids.

Experimental work on the magnetization, magnetic anisotropy and stress anisotropy of thin films which is nearly complete will be finished. New effort will be centered on placing the new ultra high vacuum system in operation; initial experiments will be concerned with the resistivity of thin films formed and annealed under ultra high vacua.

The elastic constants of Li-Mg alloys will be interpreted and prepared for publication; measurements on high temperature refractory compounds will be initiated. Experimental measurement of the thermal expansivity of KCl at $80^{\circ}K$ will be attempted.

A theoretical calculation of the conductivity tensor for specific Fermi surface geometry and for arbitrary magnetic field vector will be started. Theoretical studies of the vibration spectrum of bismuth and of lattice inharmonicity in metals will be made. The theory of the thermal expansivity of several solid types will be studied further, particularly in those cases where a negative expansivity is indicated experimentally. The suggestion from our previous work that there exists a large class of relaxation phenomena which may be treated by replacement of many transition probabilities by "sums-over-transition probabilities" will be investigated in more detail.

Contractor: Chicago, University of, Chicago, Illinois

Contract: AT(11-1)-357

Brief Title: RESEARCH ON THE SCIENCE OF MATERIALS

Investigators: Earl A. Long

Scope of Work

This contract involves support of the research of the Institute for the Study of Metals in the areas of solid state and the properties of metals. The research includes the following subjects of current active interest:

Studies on plastic deformation, lattice defects, yield point effects, and other physical measurements on single crystals of pure metals and alloys. Electrical resistivity and thermal electric power will be used as tools in these studies.

Highly precise determination of crystal structure parameters by x-ray diffraction.

Theoretical and experimental studies on the solid state including metallic systems, ionic crystals, and polymers. In particular, research on the Group V semi-metals and their alloys will be continued, using a variety of experimental techniques including acoustical absorption, microwave absorption, cyclotron resonance, and extending the range of frequencies to the sub-millimeter region and the far infrared. Most of these measurements will be done at very low temperatures to minimize the effect of lattice vibrations.

The work on semiconductors with emphasis on the problems related to impurity band conduction.

Studies on hydrodynamics and magneto hydrodynamics of liquids, ranging from water to liquid helium.

Diffusion in systems ranging from pure metals to alloys to the liquefied rare gases.

Contractor: Colorado, University of, Boulder, Colorado

Contract: AT(11-1)-377

Brief Title: METALS RESEARCH

Investigators: William F. Love

Scope of Work

One aspect of this research is concerned with the measurement of galvanomagnetic effects under the quantum limit conditions of high magnetic field and low temperatures in order to provide experimental evidence of recent theories relating to these circumstances. Current work has been carried out on the semiconductor indium antimonide and the semi-metal bismuth. The strong fields are provided by pulse discharge of a capacitor bank through solenoidal coils.

The other phase of the work is a study of the de Haas-van Alphen effect in metals by means of the pulsed field technique. The purpose of these experiments is to determine experimentally the shape of the Fermi surface in metals not amenable to measurements in the fields of ordinary electromagnets.

Contractor: Cornell University, Ithaca, New York

Contract: AT(30-1)-2150

Brief Title: SOLID STATE PHYSICS: MAGNETIC PHENOMENA

Investigators: R. Bowers and R. H. Silsbee

Scope of Work

Magnetic phenomena in solid state physics are the general subject of this research. Recent work has included a detailed analysis of the resonance spectrum of a defect produced by fast neutron irradiation of crystalline quartz. Other results show that after extended bleaching of additively colored KCl crystals, a spin resonance develops with properties difference from those of the F-resonance. The optical absorption associated with this resonance remains in the regionof the F-band. Work will continue on the study of the F-center relaxation behavior at high temperature and work in beginning on the study of relaxation times in a number of systems at low temperature.

During last year, a facility also was constructed for producing single crystals of sodium and lithium, and a laboratory was set up for galvanomagnetic measurements of metals at low temperatures. During next year, studies of the magneto-resistance of alkali metals will be continued with particular emphasis on single crystal work. Experimental studies also will be made in the area of quantum mechanical tunneling of electrons through thin layers.

Contractor: Illinois, University of, Urbana, Illinois

Contract: AT(11-1-67, Proj. No. 20

Brief Title: MECHANICAL BEHAVIOR OF DILUTE ALLOYS OF NIOBIUM

Investigators: G. M. Sinclair and C. A. Wert

Scope of Work

Studies of the thermodynamic and low temperature mechanical behavior of niobium are being made.

The Nb-N system has been studied in the temperature range from 1500°C to 2250°C. and at nitrogen pressures of 10^{-5}mm to 5 mm Hg. Results of this work have yielded the following thermodynamic data: Sievert's law has been verified, the heat of solution of nitrogen in niobium has been determined, the maximum solubility of nitrogen has been ascertained and an expression has been found relating the atom per cent nitrogen in solution to the partial pressure of nitrogen and the absolute temperature. Similar work is now progressing on the Nb-O system.

The yield behavior of niobium is being studied as a function of composition, grain size, state of stress, temperature and strain rate. The Petch equation appears to describe adequately a relation between yield stress, composition and grain size. Emphasis in current work has been on the variables temperature, strain rate and state of stress. Rate and temperature sensitivity of the yield stress appears to follow an Arrhenius relation having a stress modified activation energy. Generalizing all stress and strain values in terms of octahedral shear superimposes data obtained under different states of stress into a single $\tau_y - \Delta H$ curve.

Contractor: California, University of, Berkeley, California

Contract:

Brief Title: PHONON RESEARCH IN SOLIDS (PRS)

Investigators: Klaus Dransfeld

Scope of Work

The behavior of phonons in solids is being investigated in this project by use of microwave techniques. The research program is divided into three areas:

1. Microwave acoustic absorption and dispersion in ferrites. The acoustic Faraday rotation and absorption will be measured in Yig as a function of temperature and impurity content in hopes of producing information which will contribute to an understanding of spin lattice relaxation in ferromagnetic materials.

2. Spin-Phonon interaction in paramagnetic crystals. Relaxation measurements will be performed using recently developed hypersonic techniques and studies of heat conduction of paramagnetic crystals in external magnetic fields. The aim of this research is to develop information on the manner in which relaxation takes place. Recent experimental information does not substantiate a mechanism involving direct emission or absorption of phonons.

3. Microwave acoustic absorption in superconductors. The absorption of microwave frequencies will be investigated as the temperature of the absorption is reduced through the transition region. Recent observations on indium show an increase in absorption at just above the transition temperature followed by a decrease at lower temperature.

Contractor: Florida, University of, Gainesville, Florida

Contract:

Brief Title: THE NATURE OF ATOMIC BINDING IN DILUTE SOLID SOLUTIONS

Investigators: Albert G. Guy

Scope of Work

The Russian investigator Borovskii has noted that solute additions to transition metals in the order of 0.1 atomic per cent produce a minimum in the thermal expansion-composition curve. He has evolved a qualitative theory involving the effect of the solutes on metallic bonding to explain the observations.

The aim of the present research is to correlate the anomalous effect of alloying on thermal expansion with metallic bond strength. Although it is proposed to verify Borovskii's result, the study will encompass a much broader area than this.

Of the experimental data offered by Borovskii in support of his theory of atomic binding, those on thermal expansion appear to be the most reliable and reproducible. Therefore these data have been chosen for the initial verification of Borovskii's work. The importance of these data lies in the relation between thermal expansion and interatomic forces, since appreciable variation in thermal expansion with change in composition of a dilute solid solution must be associated with significant changes in atomic binding. If the change in thermal expansion is used as a measure of the change in atomic binding, then it would be possible to test a theory such as that of Abrahamson in which the number of d- and s-electrons in the alloying element determines the strength of binding. In view of the complexities of metallic binding it is unlikely that a theory based only on electron interactions would be completely satisfactory; however, the existing experimental evidence justifies a search for dominant, underlying regularities of the character.

The first step in the dilatometric study will be to investigate alloys of purity comparable to those employed by Borovskii. Such dilute alloys in the iron-chromium, iron-tungsten and iron-molybdenum binary systems are now on hand, and it is planned to prepare other alloys with still higher impurity levels to investigate thoroughly this possible complicating factor. Data will be obtained on a Leitz dilatometer.

Contractor: Illinois, University of, Urbana, Illinois

Contract: AT(11-1)-971

Brief Title: PROPERTIES OF INERT GAS SOLIDS

Investigators: Ralph O. Simmons

Scope of Work

This project aims to obtain quantitative information about a number of properties of the inert gas solids (Ne, A, Kr, Xe). These are cubic-close-packed crystals bound by two-body van der Waals forces, for which many calculations of properties can be made essentially from first principles. Many theoretical investigations of these materials have been reported, but accurate experimental evidence is meagre in extent, primarily because of the low melting temperatures of these solids. These crystals offer some unique advantages for detailed and fruitful intercomparison between experiment and theory.

The initial effort will be directed at the construction of a cryostat suitable for the production and manipulation of high-purity single crystals of these substances. Precise measurements will then be made by X-ray diffraction techniques of the crystal perfection, molar volume, thermal expansion coefficient, and relative intensity of high-angle Laue-Bragg intensity maxima as a function of temperature. This information should materially contribute to current investigations of crystal lattice dynamics. In addition, it should provide necessary data for the design of later experiments.

Contractor: Illinois, University of

Contract: AT(11-1)-67, Proj. No. 22

Brief Title: PROPERTIES OF MATERIALS AT LOW TEMPERATURES

Investigators: John C. Wheatley

Scope of Work

The properties of He^3 at very low temperatures are under investigation in this program. At temperatures less than $0.1^{\circ}K$ liquid He^3 exhibits many properties characteristic of a degenerate gas of quasi-particle Fermions. Measurements have been made of the spin diffusion co-efficient, the nuclear susceptibility, and the specific heat for the liquid at low pressures. The results demonstrate the degeneracy of the liquid. However, it is possible that even at $.03^{\circ}K$ and above the weakly interacting quasi-particle model is not valid. We intend to measure the thermal conductivity and the viscosity of the liquid also. In the future the velocity of sound in liquid He^3 also will be studied. All the above parameters will be measured as a function of pressure.

It is possible that at very low temperatures indeed the liquid may undergo a phase transformation into a highly correlated state. Techniques are being developed for reducing the temperature of the He^3 substantially (in order to study the question). At present no transition in specific heat has been observed down to $0.008^{\circ}K$.

Contractor: Johns Hopkins University, Baltimore, Maryland

Contract: AT(30-1)-2185

Brief Title: ESTABLISHMENT OF THE ANGSTROM AS A STANDARD FOR X-RAY WAVELENGTH AND CRYSTAL DIMENSIONS

Investigators: J. A. Bearden

Scope of Work

The extreme precautions necessary in establishing international standards often point out the inadequacy of some technique which had been accepted as proved. The establishment of the Angstrom as a standard for x-ray wavelengths and crystal dimensions has shown the inadequacy of the usual divided circle technique for the absolute measurement of angles. One expects a gradual warping and change in calibration due to aging of even the best metals, but this can be checked by periodic recalibrations which require a few months of routine measurements. A new and more serious difficulty has emerged in the present work.

Divided circles are ruled on a silver inlay because of its uniformity and small wear on the ruling diamond tool. The silver tarnishes within a few weeks on exposure to the average laboratory air and requires polishing. The polishing alters the edges of the ruling, which produces an apparent displacement of the order of a second of arc. Furthermore, in any calibration only a fraction of the rulings (usually the 5^{o} positions) are calibrated, and the position of the remaining lines are interpolated from the 5^{o} calibration curve. The above problem probably accounts for a considerable part of the disagreements in published x-ray wavelengths and crystal dimensions.

Contractor: Johns Hopkins University, Baltimore, Maryland

Contract: AT(30-1)-2543

Brief Title: REDETERMINATION OF SELECTED X-RAY EMISSION LINES

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 30 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 three thousand 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 unambiguous.

Contractor: Massachusetts Institute of Technology, Cambridge, Mass.

Contract: AT(30-1)-2574

Brief Title: SOLID STATE STUDIES IN NON-CRYSTALLINE SOLIDS

Investigators: W. D. Kingery and R. L. Coble

Scope of Work

This program is an investigation of the structure and properties of non-crystalline solids from a physical point of view. Efforts are concentrated on studies of: (1) relationship between structure and atom mobility including diffusion of oxygen in GeO and diffusion of silicon in SiO_2 glass; (2) defects in the glass structure including electrical properties of Si-silicate glasses, V_2O_5- Fe_2O_3-P_2O_5 glasses, and impurity controlled point defects in SiO_2 glass; (3) mechanical properties of glasses and polymers including damping capacity of linear and cross-linked phosphate and organic glasses, deformation and fracture of glasses in the transformation range at difference strain rates, and characteristics of ionic-linked polymers; and (4) structure and stability of non-crystalline solids formed by condensation from the vapor phase on a low temperature substrate.

Contractor: Massachusetts Institute of Technology, Cambridge, Mass.

Contract: AT(30-1)-1852

Brief Title: BASIC RESEARCH IN CERAMICS

Investigators: W. D. Kingery and F. H. Norton

Scope of Work

This program constitutes an investigation of fundamental factors affecting the properties and use of ceramics. Efforts are concentrated particularly on studies related to: (1) atom movements in ceramic materials, including oxygen diffusion in crystalline oxides (Al_2O_3, MgO, Fe_2O_3, etc.) and aluminum ion diffusion in Al_2O_2; (2) kinetics of ceramic processes, including refractory corrosion, sintering, and densification, effects of pressure on the sintering process, and crystal growth from the vapor phase; (3) development of microstructure in ceramics, including distribution of minor impurities between grains and grain boundaries, surface and interface energy relationships, and (4) effects of microstructure on properties of ceramics including creep of polycrystalline alumina at high temperatures, anelastic deformation phenomena, and electrical conductivity of oxides.

Contractor: Massachusetts Institute of Technology, Cambridge, Massachusetts

Contract: AT(30-1)-981

Brief Title: PHYSICAL METALLURGY OF UNCOMMON METALS

Investigators: John T. Norton and Robert E. Ogilvie

Scope of Work

The research programs concerned with "The Physical Metallurgy of Uncommon Metals" have been directed along three distinct avenues of study:

1. Physical Metallurgy of Uncommon Metals
2. Magnetic Behavior of Uncommon Metals
3. Crystal Chemistry of Uncommon Metals

The physical metallurgy aspects have dealt principally with solid state reactions, in particular diffusion controlled reactions. From this type of study a better understanding of the mechanisms of diffusion and the compatibility of materials will be obtained.

Study of radiation damage caused by high energy electrons has been in progress for some time. From very precise lattice parameter and resistivity measurements it is hoped that a better understanding of Frenkel defects will be obtained.

The magnetic work has been primarily devoted to the development of a theory that would explain the transition region in isomorphic pseudo-binary systems where one constitutent is ferromagnetic and the other antiferromagnetic. One such example is the UFe_2-UMn_2 system that is under investigations.

The pseudo-binaries $ReSi_2$-$TiSi_2$, $TiSi_2$-$TiSb_2$ and $ReSi_2$-$ReAl_2$ are under investigation from the standpoint of space filling, lattice parameter, electron-atom ratio and electronic configurations. It is expected that a better understanding of the C11, C40 and C54 type structures will be obtained.

Contractor: Massachusetts Institute of Technology, Cambridge, Massachusetts

Contract: AT(30-1)-2592

Brief Title: NEUTRON DIFFRACTION STUDIES OF LOW TEMPERATURE PARAMAGNETIC ALIGNMENT IN SOLIDS

Investigators: C. G. Shull

Scope of Work

Polarized neutron radiation is to be used in studies of low temperature paramagnetic alignment as a means of determining the magnetic characteristics of paramagnetic 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. In the experiments, single crystals of paramagnetic salts or metals (possessing very low Neel or Curie temperatures) are to be subjected to high magnetic fields while at liquid helium (or lower) temperature and the resulting coherent scattering with polarized radiation is to be examined. New experimental techniques for combining the polarized beam, low temperature and high magnetic field aspects are being developed. These same techniques will be useful in later exploration of nuclear alignment in crystals.

Contractor: Michigan College of Mining and Technology, Houghton, Michigan

Contract: AT(11-1)-916

Brief Title: STRUCTURE AND PROPERTIES OF SOLID SOLUTIONS

Investigators: A. A. Hendrickson

Scope of Work

The main purpose of this investigation is to determine the cause or causes of solid solution hardening in particular alloys. The method of attack involves the correlation of the strength properties of solid solutions with current theories of solid solution strengthening.

The experimental program involves the following measurements: (1) The effect of crystal perfection on the strength of Ag base solid solutions (2) The dependence of the critical resolved shear stress of Ag base alloy single crystals as a function of solute content, testing temperature and strain rate and (3) Yield point effects in Ag base solid solutions.

Contractor: Minnesota, University of, Minneapolis, Minnesota

Contract: AT(11-1)-1009

Brief Title: ANOMALOUS RESISTIVITY CHANGE IN Pd-Cu AND Pd-Ag ALLOYS

Investigators: Morris E. Nicholson

Scope of Work

An anomalous decrease is observed in the resistivity of Au-Pd, Cu-Pd, and Ag-Pd alloys as a function of plastic deformation. Although this behavior has been studied in some detail a thorough investigation has not been made. The most complete investigation of this phenomena was made by Jaumot and Sawatsky. However, there is still considerably speculation regarding the nature of this change in resistivity.

The proposed study involves: (a) detailed study of the change in resistivity at liquid nitrogen temperatures as a function of working at these temperatures; (b) detailed studies of the resistivity as a function of temperature after room temperature cold working; (c) a determination of the magneto resistivity of the alloys to determine if there is any anisotropy in the resistivity; (d) a Hall effect and magnetic susceptibility study to determine whether or not the electronic structure of the alloys have been altered by cold work.

In order to obtain further evidence regarding the nature of the defects causing the anomalous resistivity change, resistivity will be measured after low temperature annealing operations. Elastic constant measurements will also be made as a function of cold work to determine whether or not a change in resistivity is an electron-phonon interaction.

Before the completion of the research it is anticipated that thin film studies using electron microscopy and the Hirsch technique will be used to determine whether or not any unusual dislocation morphologies exist which might cause the anomalous resistivity behavior.

Contractor: Notre Dame, University of, Notre Dame, Indiana

Contract: AT(11-1)-713

Brief Title: X-RAY INVESTIGATION OF MACRO AND MICRO RESIDUAL STRESS

Investigators: B. D. Cullity

Scope of Work

This research is concerned with macro and micro residual stress in metals and with its measurement by x-ray diffraction. Nickel, plastically strained, is the particular metal under investigation. Macrostress is being measured by diffraction line shift and microstress by Fourier analysis of line shape. The relaxation of these stresses during isothermal annealing will be studied, as well as their effects on certain magnetic properties.

Another material being investigated is silicon steel. It is known that magnetic hysteresis losses in this material are markedly higher after plastic stretching. X-ray measurements of residual macrostress after plastic stretching are being made in order to find the cause of this effect. A phenomenological theory of the development of residual compressive macrostress (observed in many metals) has been formulated, which accounts for the main features of the phenomenon.

Contractor: Oklahoma, University of, Norman, Oklahoma

Contract: AT-(40-1)-2507

Brief Title: X-RAY ABSORPTION EDGE SPECTROMETRY

Investigators: Charles G. Dodd

Scope of Work

The theoretical principles and experimental requirements of x-ray absorption-edge spectrometry with respect to its use in chemical analysis have been developed during the past two years. These principles and experimental requirements will now be applied to the development of precise methods of analysis for selected chemical elements throughout the periodic table. Constant potential x-ray sources and custom-designed apparatus will be employed to measure x-ray mass-absorption-coefficient "edge jumps" with adequate precision. Chemical analytical facilities will be developed for independent analysis of standard samples. X-ray absorption-edge structure phenomena will be investigated further.

Contractor: Pennsylvania, University of, Philadelphia, Pennsylvania

Contract: AT(30-1)-2395

Brief Title: OPTICAL AND MICROWAVE SPECTROSCOPY OF SOLIDS

Investigators: E. Burstein

Scope of Work

The research carried out on this program falls into three major areas:

a) Infrared Lattice Vibration Spectra

Room temperature reflection measurements were obtained for LiH over the range of 2 to 50 microns. The data yielded a value of 600 cm^{-1} for the transverse optical vibration frequency and a value of 1120 cm^{-1} for the longitudinal optical vibration frequency. When combined with available values for the low and high frequency dielectric constants one obtains a value of 0.52 e for the Szigeti dynamic effective ionic charge. This relatively low value of the effective charge is attributed to the large charge deformability of the H ion and to large "overlap" effects. A similar study will be carried out for LiD and the measurements will also be extended to low temperatures.

b) Electron Tunneling in Semiconductor and Metals

An unsuccessful attempt was made to see "de Haas-van Alphen" type oscillators in the I vs V or I vs H characteristics of several InAs diodes using steady magnetic fields up to 30,000 gauss and pulsed magnetic fields up to 125,000 gauss. The decrease in tunneling current for H parallel and for H perpendicular to the junction was found to be in reasonable agreement with theory. The use of electron tunneling in superconductors for the detection of millimeter and submillimeter-waves was proposed and a calculation was made, using detailed balance, of the optical recombination lifetime of excited carriers in electrons and holes. An experimental investigation of the lifetime of excited carriers in superconductors using electrical as well as optical injection techniques is now under way.

c) Landau Level Investigations of Compound Semiconductors

Although p-type PbTe satisfies the criteria for observing Azbel-Kaner cyclotron resonance, an effort to observe such resonance at 8 mm was unsuccessful, presumably due to inadequately prepared surfaces. However, experiments on the de Haas-van Alphen effect using Shoenberg's

impulsive method were successful and well defined oscillations in the magnetic susceptibility were observed. This is the first time that such experiments have been carried out for a semiconductor. Measurements of oscillations in magnetic susceptibility have the advantage of greater simplicity over the measurements of oscillation in transport properties, such as Hall effect and magneto-resistance, as they do not require electrical contacts and do not include the current as an additional parameter. Complete measurements are being obtained for PbTe as well as for PbS and PbSe. The investigation of Azbel-Kaner resonance in these materials will also be continued.

Contractor: West Virginia University, Morgantown, West Virginia

Contract:

Brief Title: VOLUME MAGNETOSTRICTION IN FERROMAGNETIC MATERIALS

Investigators: Arthur S. Pavlovic

Scope of Work

The chief goal of this program is to obtain volume magnetostriction and magnetocaloric measurements on a number of magnetic materials; data will be used to verify current theories of magnetism.

During the intial stages of the program research will include experimental determination of the volume magnetostriction of iron, gadolinium, and various magnetic alloys over a broad temperature range with high accuracy. Of particular interest will be data obtained at temperatures close to the Curie Point. Longitudinal magnetrostriction and the magnetocaloric effect will be determined in gadolinium. Results will be reviewed in terms of currently proposed interaction curves (a measure of the magnitude of the variation of exchange force with interatomic distance) in order to establish the validity of magnetic theory.

Section III

INTERACTION OF RADIATION WITH MATTER

Section III-A

Nature and Behavior of Defects

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

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

Brief Title: RADIATION DAMAGE IN CRYSTALLINE SOLIDS

Investigators: A. Sosin and F. H. Eisen

Scope of Work

Studies of radiation damage in solids directly yield information on the effects of radiation on materials, but also provide a sensitive tool for investigating defects in solids. It is the objective of this project to study the production of defects in crystalline solids by radiation and to attain an understanding of their structure, their interactions with each other and with impurities and dislocations, their effect on the physical properties of solids, and their recovery kinetics. The materials chosen for study are metals, metallic alloys, and semiconductors.

Recent work on this project typical of the proposed future efforts includes the following:

a) A detailed study of the energy dependence of damage rate at $4.2^{\circ}K$ and on subsequent recovery in copper and dilute copper alloys. This study has revealed the inadequacy of a step-probability ejection function for damage near threshold energy and an unexpected energy dependence of recovery. A theory to explain these results based on strong focusing has been explored.

b) Companion studies of recovery of dilute copper alloys in the range above $80^{\circ}K$. Additional recovery stages are introduced by the alloying element. The energies, magnitudes, and kinetics of these stages bear on the interpretation of radiation effects in pure copper as well as the nature of impurity-defect interaction.

c) Elastic modulus and internal friction changes due to irradiation. It has been shown that these changes cannot be simply ascribed to pinning of a single type of dislocation by point defects and, furthermore, that the recovery to pre-irradiation values proceeds at unexpectedly high temperature, implying a strong dislocation-defect interaction.

d) Electron irradiation damage and recovery has been extensively studied in n-type InSb. A model for recovery, including electrical interaction has evolved. The threshold energy for displacement, about 6 ev, is unusally low.

Contractor: Brookhaven National Laboratory, Associated Universities, Inc. Upton, Long Island, New York

Contract: AT(30-2-Gen-16

Brief Title: FISSION FRAGMENT EFFECTS IN SOLIDS

Investigators: J. Felsch, O. Kammerer, D. H. Gurinsky

Scope of Work

Electron microscopy techniques are being used in a comprehensive investigation of the changes produced in solids by the passage of fission fragments and other highly energetic particles.

In thin evaporated films of Al, Cu, Ge, Ag, Au, Pt and U in the thickness range of <100Å to ≤250Å well defined tracks are seen. In the metals of higher atomic number and density the tracks are increasingly prominent and indicate a higher rate of energy transfer from the fission fragment to the matrix atoms. The permanent changes produced in the matrices studied seem to be due to the vaporization of matrix-atoms along that portion of the fragment path where energy transfer is greatest, subsiding to a melting in the region where the energy transfer is less. An attempt is being made to isolate the origin of fission events in order to study the region from the origin to the area where vaporization occurs. The former is the region in which energy loss is due to electron interaction, according to theory.

This work will include the study of the same phenomona in single crystal films, and in electrolytically thinned bulk foils thus covering the thickness spectrum from <50Å to 25,000Å.

The future aspects of this investigation will include a study of the end of the range of high energy alpha particles, fast neutrons, and the products of the Li^6 and B^{10} disintegrations. The objective is a better understanding of the interaction of high energy particles on metallic and non-metallic matrices.

Contractor: Brookhaven National Laboratory, Associated Universities, Inc., Upton, Long Island, New York

Contract: AT(30-2)-Gen-16

Brief Title: RADIATION EFFECTS

Investigators: G. J. Dienes, G. H. Vineyard, A. C. Damask, D. T. Keating, P. W. Levy, A. N. Goland, D. B. Rosenblatt, T. B. Flanagan, L. C. R. Alfred, B. Mozer, F. E. Fujita, J. Jach

Scope of Work

One of the major research activities in solid state physics is the study of defects in crystals. Radiation effects and other departures from perfect periodicity are under investigation with many diverse techniques.

Optical, Ultrasonic and Magnetic Resonance Studies of Insulators

Optical measurements on alkali halides and other insulators are yielding important basic information about the number and character of radiation induced defects. Coloring measurements on reactor and gamma-ray irradiated alkali halides can be used to determine the concentration of defects produced by reactor irradiation. Curves of F-center coloring vs. gamma-ray dose rise rapidly below 10^6r and then level off to a constant slope. If a gamma-ray coloring curve is interrupted with a short reactor irradiation a stepwise increase is introduced in the coloration. In this way it is found that the reactor irradiation markedly increases F,V,M,R, and other bands with slope of the gamma-ray coloring curve remaining the same before and after short (30 min.) reactor irradiation. From the stepwise increase one can compute the number of vacancies produced. Quite good agreement is found with the Kinchin-Pease and Seitz-Koehler theories.

Stepwise annealing studies of the reactor-induced absorption bands in Al_2O_3 at 6.02, 5.35, and 4.85 ev have been completed. In one variant of these experiments, previously colored samples are heated for a fixed period at each of successively higher temperatures and the optical absorption is measured after each anneal. In another variant, after each anneal the crystals are recolored with gamma-rays until equilibrium coloring is attained. The same principal defect removal stages appear in both variations of this method. From the gamma-ray recoloring process itself further information about electronic changes is obtainable. A clear cut interpretation of the recoloring process has not yet been achieved. Similar experiments on fused silica colored by reactor irradiation have shown that all of the color removed by heating to 270°C can be restored by exposure to gamma rays. This indicates that this part of the annealing is purely electronic. Annealing experiments at higher temperatures are in progress. This is a long term study because high gamma-ray exposures are required to separate out the electronic component.

to the conventional theory of thermal spikes 16% of the gray tin should have been transformed to white tin during this particular irradiation. The experimental results indicate strongly, therefore, that the theory of thermal spikes needs considerable revision.

An attempt is being made to isolate and study radiation enhanced nucleation in alloys. The iron-carbon system was selected for investigation because there is no evidence that radiation can enhance interstitial migration. Iron containing 0.01 wt.% carbon was irradiated in the BNL reactor at different times and temperatures, and the amount of carbon in solution was measured by torsion pendulum internal friction. Regardless of the extent of precipitation prior to irradiation, no increase of carbon in solution was observed, which indicates that the irradiation does not tend to dissolve precipitates. Subsequent annealing showed that the irradiation always accelerated the disappearance of carbon from solution by about three orders of magnitude over the thermal rate. The decay curves are all second-order with an activation energy that is the same as that for self-diffusion of carbon in iron, in disagreement with the reaction kinetics and activation energy for thermal precipitation. It is not known yet whether this accelerated disappearance of carbon from solution arises from enhanced nucleation or an interaction of the carbon with radiation induced defects. Work is continuing on this system by resistivity, calorimetric, and electron microscope techniques.

Mössbauer Effect

On the basis of theoretical work and some preliminary experiments a series of investigations using the Mössbauer effect has been planned involving:

a) the magnetic properties of various ferromagnetic alloys of iron, tin, and perhaps of nickel, as well as compounds such as Fe_4N;

b) the ferroelectric properties of certain crystals in an attempt to determine electric field gradients and electric quadrupole moments;

c) the precipitation of Ni in Cu-Ni alloys, if a Mössbauer effect actually exists for Ni^{61};

d) localized vibrational modes of impurities in metals (also to be correlated with inelastic neutron scattering studies).

Chemical Effects of Irradiation

Studies of the effect of radiation on the chemical activity of solids are continuing. The thermal decomposition of $NaBrO_3$ is under investigation. Gamma-ray irradiations cause a marked increase in decomposition rates. Neutron irradiations initially cause a large increase in decomposition rates but upon prolonged irradiation the rate decreases. For example, two day irradiations cause a tenfold rate increase, but $NaBrO_3$ exposed for four weeks decomposes at the rate found for non-irradiated crystals. However, during a four week irradiation, an appreciable fraction of the original mass has disappeared dut to radiation decomposition. These observations, as well as those made previously on $KBrO_3$,

Preliminary paramagnetic resonance studies of irradiated crystals have shown a great deal of promise. Electron spin resonances, suitable for detailed study, have been found in a number of irradiated crystals (KN_3, Al_2O_3, TiO_2, $NaBrO_3$, $NaClO_3$). For example, a 5 line resonance system, attributable to N_4^- has been observed in gamma-ray irradiated KN_3. This system appears to decay at the same rate as one of the radiation induced color centers. Two other radiation induced systems are formed by gamma-ray irradiation at liquid nitrogen. One is suggestive of N_2^- ions and the other apparently involves only a single nitrogen atom. As another example, a single spin resonance appears in gamma-ray irradiated Al_2O_3 which has a hole-like character with $g \approx 2.01$. High sensitivity measurements on TiO_2 disclosed at least ten resonance systems induced by gamma-ray irradiation at liquid nitrogen.

An in-pile ultrasonic experiment has been carried out successfully. The ultrasonic attenuation and velocity changes in α-quartz during reactor irradiation have been measured. Velocity changes were very small but large increases in attenuation were found. After temperature equilibrium is reached, the attenuation increases steadily with two well defined peaks superimposed on the curve. After approximately one week in the reactor, the attenuation reaches its saturation value which is changed only slightly by an additional week of irradiation.

X-ray Studies

The work on radiation effects in diamond, a purely covalent crystal, continues. Samples have now been irradiated in the Materials Testing Reactor up to an integrated fast flux of 1.4×10^{21} nvt. The density of these irradiated diamonds was found to be 1.96 gm cm^{-3}, i.e. the density is less than that of graphite (2.25 gm cm^{-3}) and represents a decrease of 44% in the density of diamond. The density varies linearly with irradiation dose up to this very high exposure. For such heavy irradiations the diamond has a glass like or amorphous structure but retains its external crystalline features. The hardness is approximately that of the hardest nitrided steels. Because of its amorphous structure, its physical properties, such as hardness and x-ray patterns are independent of orientation. It is surprising that such a heavily irradiated and badly distorted solid holds together at all; it is even more surprising that it is very stable. Annealing studies show that for temperatures of 1000°C or more a further 5% decrease in density occurs while for lightly irradiated diamonds annealing produces an increase in density (i.e. recovery to daimond). Final interpretation must await further work but it is clear that we are dealing here with a very unusual form of solid carbon.

Effect of Irradiation on Solid State Reactions

There has been considerable speculation about the production and properties of thermal spikes during irradiation, but no clear cut experimental evidence has been found for or against the existence of such spikes except in fissionable materials. The gray-to-white tin transformation is a highly favorable process for indicating the presence of thermal spikes. Gray tin was irradiated at 0°C in the reactor in an effort to produce white tin as a result of localized heating caused by thermal spikes. The irradiated powder was compared to an unirradiated specimen by means of x-ray studies at low temperatures. No significant change was found in the amount of white tin present as a result of irradiation. According

are in accord with the conjecture that the increased decomposition rates are related to enhanced diffusion occurring in the irradiated materials. Experiments have also been started on manganous oxalate dihydrate.

An investigation of the effect of prior reactor irradiation on the gas adsorption properties of gamma Al_2O_3 has been in progress for some time. Extensive data are now on hand for hydrogen adsorption on this material. Hydrogen adsorption is decreased by irradiation of the solid and the shapes of the isotherms are altered. The results can be explained by one of two hypotheses. The first is that the packing gas molecules on the solid surface is changed after the solid is damaged by radiation. The other possibility is that some gas is released during irradiation, which first adheres to the solid but is replaced by hydrogen as the latter is adsorbed on the surface during the course of an experiment. Although the second hypothesis is difficult to accept there is some evidence supporting it. The shape of the adsorption isotherms is consistent with a simple replacement process, and, in addition, mass spectrometer analysis of the gas obtained during a run shows that nitrogen is released into what is originally pure hydrogen. Chemical analysis of the γ-Al_2O_3 (a commercial catalyst) shows that traces of nitrogen are present in this material. Further work is needed before a clear cut choice can be made between these two hypotheses.

Theory

Machine calculations of radiation damage dynamics have given excellent data. A successful scheme has been developed for taking movies of various damage events and processes. Low and moderate-energy damage events and the properties of a number of simple defects in copper are now well understood. The interstitial has been shown to possess only tetragonal symmetry, instead of full cubic symmetry as was generally supposed. The crowdion has been shown to be unstable, but a dynamic crowdion has been shown to propagate along both <110> and <100> directions. Collision chains are prominent in these directions; they focus at low energies and defocus at higher energies. Above threshold, the chains transport matter, as well as energy, and produce an interstitial at a distance. Various interstitial-vacancy pairs have been examined and are found to be stable only beyond minimum separations, which depend very much on orientation.

The interaction of simple defects during annealing is being investigated. Important results have been obtained for impurity-vacancy interaction, for divacancy formation, for interstitial impurity interaction and diinterstitial formation. The differential equations describing these interactions and the simultaneous annealing of defects are generally non-linear and cannot be solved in closed form. A successful technique has been developed whereby the validity of physically important approximations can be delineated by comparison with complete analogue computer solutions. These theoretical results have a direct bearing on the interpretation of quenching and radiation damage experiments.

Contractor: Brown University, Providence, Rhode Island

Contract: AT(30-1)-1880

Brief Title: RADIATION DAMAGE STUDIES IN SOLIDS; NUCLEAR RESONANCE ABSORPTION TECHNIQUE

Investigator: P. J. Bray

Scope of Work

The initial objective of this project was to demonstrate the utility of the technique of nuclear magnetic resonance in studying the effects of irradiation on materials. This objective has been realized through both quantitative and qualitative observation. In particular, colloidal lithium and gaseous fluorine have been found and identified as irradiation products trapped inside single crystals of pile irradiated lithium fluoride. Quantitative measurements of the extent of damage in many alkali halides have been made.

The examination of materials prior to their irradiation has initiated an important study of glasses by this technique. Similarly, contributions have been made to the understanding of the physical, chemical, and crystallographic properties of several materials.

In the coming year investigations of pile irradiated alkali halide single crystals will be the major effort. Emphasis will center on comparisons among compounds and among different amounts and conditions of irradiation. As these alkali halide studies approach completion more emphasis will be placed on the investigation of effects due to other forms of irradiation and effects in other types of materials. The study of irradiated semiconductors will be an important new project in the coming year.

Contractor: Brown University, Providence, Rhode Island

Contract: AT(30-1)-2024

Brief Title: RADIATION DAMAGE STUDIES USING THE TECHNIQUES OF ELECTRON-SPIN PARAMAGNETIC RESONANCE

Investigators: P. J. Bray and A. O. Williams, Jr.

Scope of Work

During the fourth year of the research effort under Contract AT(30-1)-2024, studies of radiation damage in three types of solids will be pursued. These are alkali halide single crystals, glasses, and alkali azides.

Of the alkali halides, LiCl, LiBr and LiI will receive the most attention in view of the unexpected results obtained from LiF. It is believed that, unlike LiF, these materials may be more accessible to optical bleaching and absorption measurements, thus giving wider scope and greater precision to the basic electron-spin resonance measurements.

Investigation of radiation-induced defects in glasses will receive considerably more attention during the current year. In view of the intense and well-resolved hyperfine structures that have been observed, it is expected that considerable progress will be made toward identifying the paramagnetic defects. The nature of these defects appears to be strongly dependent on the compositions of the glasses studied; the direction thus indicated for further work will be pursued. Optical absorption measurements are also planned.

Preliminary investigations of neutron-irradiated crystals of KN_3 have revealed two kinds of defects, one stable, the other unstable, at room temperature. The latter gives rise to a well-resolved hyperfine structure. It appears that good single crystals of the azides will be needed; attempts are currently being made to grow these from aqueous solution.

All of the above areas of research will benefit from two projects that are to be completed during the current year: construction of a well-regulated electric oven for thermal and simultaneous thermal-optical annealing experiments; establishment of a procedure for irradiation, handling and observation of materials at liquid nitrogen temperature.

Contractor: Carnegie Institute of Technology

Contract: AT(30-1)-1828

Brief Title: RADIATION EFFECTS IN SOLIDS

Investigators: A. Halperin

Scope of Work

This program consists of a diversified study of radiation effects. Research is being performed in the following specific areas:

1) Mechanics of defect formation and low-temperature annealing in the alkali halides

2) The effect of radiation on thermal expansivity in NaCl

3) Structural sensitivity of ionic crystals to defect production

4) Effect of deformation and irradiation on ionic and electronic conductivity

5) Paramagnetic resonance effects

6) Effect of irradiation on catalytic activity

7) Field and ion emission study of radiation effects in tungsten

Contractor: Connecticut, University of, Storrs, Connecticut

Contract: AT(30-1)-2047

Brief Title: INVESTIGATIONS OF RADIATION EFFECTS IN METAL OXIDES AND AZIDES BY ELECTRON SPIN RESONANCE

Investigators: Otis 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. New spin resonances are obtained in α-Al_2O_3 by gamma ray irradiations, by reactor irradiations, and by 10^6-r gamma ray irradiations at LNT following higher temperature reactor irradiations. In clear Linde rutile (TiO_2) valence states of paramagnetic impurity ions are changed and new spin resonances are observed after gamma ray or uv irradiations at 77°K. Experiments on Corning 7943 fused silica have indicated that spin resonances result from the quenching of flame-softened fused silica in water. This quenching also causes enhancement in the ESR absorption obtained by subsequent uv irradiation. A 10^6-r gamma ray irradiation of the 7943 at 300°K causes additional ESR lines. At least three paramagnetic centers are detected in potassium azide after a gamma ray irradiation of 10^6r at 77°K. All of these centers show hyperfine interactions with nitrogen nuclei. Symmetry properties, growth data, annealing behavior, line widths, relaxation times, g-values, fine structures, hyperfine structures, and doped crystals are being studied to enable interpretations of these various radiation effects. Correlative studies on the same or similar samples by optical methods are being performed by P. W. Levy of the Solid State Physics Group at Brookhaven National Laboratory. Other crystalline materials believed favorable for learning about radiation damage and annealing mechanisms are being examined, and new experimental techniques are being developed.

Contractor: General Mills, Inc., Mechanical Division
Minneapolis, Minnesota

Contract: AT(11-1)-722

Brief Title: SURFACE BOMBARDMENT STUDIES

Investigators: G. K. Wehner

Scope of Work

I. SPUTTERING OF SINGLE CRYSTALS

Low index planes of metal single crystals are bombarded with Hg or noble gas ions up to 1 kev energy under well controlled conditions in a low pressure plasma. Atoms are then ejected or sputtered in certain preferred crystallographic directions. The study of this phenomenon for different ions and metals, at various bombarding energies and targets temperatures, furnishes a wealth of information on details in the sputtering process, on the energy transfer in the lattice, focusing collisions, and on crystal structure changes under ion bombardment. Results from this work are of much interest in many radiation damage problems.

II. SPUTTERING YIELDS FOR HYDROGEN- AND HELIUM-ION BOMBARDMENT

Supplementing the sputtering yield measurements under Hg^+, Ar^+ and Xe^+ ion bombardment (collected under an ONR contract), the sputtering yields for H^+ and He^+ are determined for various metals in the energy range up to several kev. There are indications that the basic process in sputtering of heavy metals by light ions is basically different from the reverse case. Hydrogen and He data are needed in thermonuclear fusion research, in astrophysical problems ("solar-wind" bombardment) and for establishing a universal sputtering law.

Contractor: Hanford Atomic Products Operation, General Electric Company, Richland, Washington

Contract: W-31-109-Eng-52

Brief Title: MECHANISM OF GRAPHITE DAMAGE

Investigators: I. Myers and W. C. Roesch

Scope of Work

The purpose of this study is to acquire basic knowledge of radiation damage and annealing effects for reactor graphite.

Preliminary experiments at room temperature have been carried out on graphite to determine the minimum energy required of Van de Graaff generated electrons to produce a displacement resulting in a change in resistivity.

Measurements of the minimum energy for displacement, of resistivity change, and of length change under electron bombardment and of annealing rates for residual effects will be completed for a few types of graphite as functions of temperature. These effects will be related to those observed in neutron bombardment.

Contractor: Hanford Atomic Products Operation, General Electric Company, Richland, Washington

Contract: W-31-109-Eng-52

Brief Title: RADIATION EFFECTS ON METALS

Investigators: J. C. Tobin

Scope of Work

The purpose of this project is to study how initial imperfection concentrations such as impurity atoms and dislocation densities influence the damage ascribed to neutron bombardment of metals and to determine how the accumulated damage is changed by thermal annealing treatments.

Damage recovery stages have been characterized for Zr, Ti, Fe, Ni, Mo, and Cu on the basis of activation energy. Reaction orders and rate constants were determined for Zr, Fe, Ni, Cu, and Mo. Mechanical tests were made on these specimens.

The damage invoked in molybdenum single crystals with controlled impurity contents and known histories will be characterized as a function of various total exposures. Pre- and post-irradiation transmission electron microscopy, x-ray lattice parameter and line width measurements, and various mechanical property tests will be used in determining deformation mechanisms and changes in structure of these crystals.

Contractor: Houston, University of, Houston, Texas

Contract: AT-(40-1)-2573

Brief Title: SPUTTERING BY ION BEAMS

Investigators: H. K. Reynolds

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 will be measured as a function of the energy and nature of the bombarding ion, its angle of incidence on the target. The energy range to be 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. (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 Institute of Technology, Chicago, Illinois

Contract: AT(11-1)-90, Proj. No. 9

Brief Title: INVESTIGATION OF ENERGY TRANSFER PROCESSES BY FLASH PHOTOLYSIS

Investigators: Leonard I. Grossweiner

Scope of Work

Optical bleaching of F centers in x-rayed and additively colored KCl has been studied at 77°K with pulse light techniques. Constant "F light" incident on the colored crystal establishes a photostationary equilibrium between F and F' centers. The application of a high intensity light flash of appropriate spectrum displaces the equilibrium to either direction. The return to equilibrium is exponential in time, with a rate controlled by the intensity and spectrum of the continuous light, but not depending on the F center concentration or the method of coloration. A saturation of the extent of bleaching at high pulse light intensities and a lower bleaching efficiency for additively colored crystals indicates that the distribution of F centers is significant in low-temperature bleaching. Irradiation of the fluorescein series dyes in their visible absorption bands excites metastable triplet states which decay by the bimolecular reaction of triplet molecules. A rapid reaction of phenol with triplet eosin dye is shown by the retardation of the rate of aerobic photobleaching and an acceleration of the rate of triplet disappearance. The primary photochemical reaction between phenol or phenolate ion with the triplet dye produces a phenoxy free radical and a semiquinone dye radical, which disappear in second-order processes. The competition between physical quenching of the triplet and charge-transfer chemical reaction can be explained by spin-conserving processes.

Contractor: Illinois, University of, Urbana, Illinois

Contract: AT(11-1)-182

Brief Title: RESEARCH ON RADIATION DAMAGE

Investigators: J. S. Koehler

Scope of Work

The 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 magnitude 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 possibly 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.

Contractor: North Carolina, University of, Chapel Hill, North Carolina

Contract: AT-(40-1)-2577 - Modification No. 1

Brief Title: RADIATION DAMAGE AND OTHER STUDIES BY MEANS OF A VAN DE GRAAFF ACCELERATOR

Investigators: Paul E. Shearin

Scope of Work

That portion of the contract concerned with solid state physics involves the use of a two-million-volt Van de Graaff Accelerator in radiation damage studies. Radiation damage in pure crystalline metals and simple semiconductors whose structures are well known is produced by bombardment with electrons or deuterons. Bombardments are done at low temperatures (around $10^{\circ}K$) in order to preclude annealing effects. Some specific studies include:

(1) Study of radiation effects and annealing effects in pure copper.
(2) Study of annealing kinetics after bombardment as a function of added impurities.
(3) Study of radiation effects and annealing effects of aluminum.
(4) Study radiation effects in semiconductors of varying purity and dislocation content such as Germanium.
(5) Initiate study of instantaneous concentration of bombardment-induced damage sites.
(6) Initiate measurement of annealing kinetics in bombarded AlCo of AlNi.
(7) Initiate studies of defects in metals by condensing them on substrates at liquid helium temperatures.

Not all of these studies can be completed within the current contract period, but constitute a long-term program.

Contractor: Northwestern University, Evanston, Illinois

Contract: AT(11-1) 89, Proj. No. 11

Brief Title: A 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. IBM 650 and 709 digital computers are used in the analysis of various aspects of this research.

Recently a study of the annealing spectrum of irradiated gold has been carried out from $10^{\circ}K$ up to complete recovery. Differences were observed in the annealing behavior between gold and copper for comparable irradiations and specimen purity. The activation energy for interstitial migration appears to be lower in gold than in copper and more clustering as compared to recombination occurs in gold, than in specimens of copper of comparable purity. A careful comparison is under way with the annealing characteristics of quenched gold in order to distinguish those processes due to lattice vacancies. Other studies involve damage production and recovery for a wide range of electron energies. Crystal orientation effects and volume change studies are in progress.

Contractor: Purdue University, Lafayette, Indiana

Contract: AT(11-1)-125

Brief Title: BASIC RADIATION DAMAGE STUDIES

Investigators: Hubert M. James

Scope of Work

The work of this project is aimed toward identification of radiation-induced defects and their associated electronic states, and toward obtaining information about the processes by which lattice defects are formed, diffuse and recombine when a semiconductor is exposed to energetic radiation. It has become clear from past studies that the nature and behavior of the defects depend not only on the temperature but also on the energy and intensity of irradiation and on the type (n-or p-) of the crystal. It appears that the simplest conditions that can be attained are those produced by irradiation at liquid helium temperature by electrons with energies not too far above the threshold for damage. A major portion of our program is concerned with measurements on crystals irradiated under these conditions. Studies are being made of the rate of introduction of damage, thermal annealing, radiation annealing and stored energy release as functions of irradiation energy and Fermi-level. At higher temperatures we are investigating the ways in which the number and types of defects produced per incident electron depend on radiation intensity and temperature, and the presence of absorbed hydrogen. Magnetic resonance equipment for studies of the properties of the defects as paramagnetic centers has been constructed, and a program of observations is getting under way. The resonance results will be carefully correlated with other properties of the defects, including their rates of production and anneal.

Contractor: Rensselaer Polytechnic Institute, Troy, New York

Contract: AT(30-1)-1995

Brief Title: RADIATION DAMAGE IN SOLIDS

Investigators: Edmond Brown

Scope

Atomic configurations around point defects in copper are being studied theoretically on the basis of a simple model. The spectrum of activation energies associated with the recombination of close pairs is one of the objectives of this investigation. The model makes use of a Born-Mayer repulsive interaction between atoms as well as a volume dependent cohesive energy, in addition to an elastic energy associated with the distant region. The atomic positions and associated configurational energy for stable and unstable equilibrium configurations are determined by an iterative procedure on an IBM 704 computer.

The model does not treat explicitly the energy associated with the correlated redistribution of electrons in the vicinity of the defects. This term requires for its proper treatments a full quantum mechanical many-body perturbation theory. Present theories of such correlated motions are not suited to numerical calculations. It is our hope to calibrate this term by making use of experimentally determined energies associated with diffusion.

Contractor: Wayne State University, Detroit, Michigan

Contract:

Brief Title: ELECTRON PARAMAGNETIC RESONANCE STUDIES OF RADIATION EFFECTS IN SOLIDS AND CHEMICAL COMPOUNDS

Investigators: Yeong-Wook Kim

Scope of Work

The primary objective of this research is the study of radiation effects using the techniques of electron paramagnetic resonance absorption. The effects of radiation will be investigated on the following materials:

1) Li compounds: research will be concerned with the thermal annealing characteristics of defects, possible formation of metal grains and their characteristics, and correlation of defects with the nature of the compound.

2) Free Radicals: the effect of varying temperature and irradiation conditions in the nature of the free radical species will be studied. Initial work will be performed using 1,1-diphenyl-2-picryl hydrazyl(DPPH) and its derivatives.

3) Antiferromagnetic materials: the effects of radiation on the transition temperature for antiferromagnetism will be correlated with the dependence of antiferromagnetism on lattice disorder. Preliminary studies will be performed with Cr_2O_3.

Section III-B

Effect of Radiation on Properties and Processes

Contractor: Argonne National Laboratory, Lemont, Illinois

Contract: W31-109-eng-38

Brief Title: IRRADIATION EFFECTS

Investigators: B. Loomis, K. Merkle, H. Hart

Scope of Work

The main effort of this program has been concerned with the nature of the damage and defects produced on neutron irradiation of fissionable materials. Two programs are currently under study: a) kinetics of fission gas accumulation in uranium and uranium alloys; and b) electron transmission microscopic study of fission fragment damage in the foils of Al Au, and other materials. Some interesting results have been obtained from post irradiation annealing studies on the effects of such variables as initial structure, purity, phase distribution, and mechanical properties on high-temperature swelling. These, it is hoped, will be correlated with swelling behavior on irradiation in situ.

Plans are being formulated for the installation of a low-temperature irradiation facility in either CP-5 or the Juggernaut reactor.

Contractor: Argonne National Laboratory, Argonne, Illinois

Contract: W-31-109-eng-38

Brief Title: RADIATION DAMAGE TO VARIOUS SOLID MATERIALS

Investigators: W. Primak

Scope of Work

The general goal of the program is a more thorough understanding of the mechanism of damage and of the influence of various solid state structures on sensitivity to damage. Radiation-induced dimensional changes are being studied in various solid materials using interferometry, precision density measurements, strain-birefringence, and capacity measurements. Thermal annealing studies of the radiation-induced defects are also underway.

The fast neutron induced expansions in crystals of SiC have been measured for directions along the optic axis and perpendicular to it. The frequency factor for thermal annealing of fast-neutron induced density changes in vitreous silica has been determined. A new constant temperature facility in the research reactor is being used to obtain more quantitative data on radiation effects.

Low energy heavy ion bombardment of surfaces is planned in order to study sputtering and radiation damage. A versatile low energy accelerator for such studies is being acquired. As a prelude to this work, new techniques of surface observation and measurement are being developed.

Contractor: Arizona State University, Tempe, Arizona

Contract: AT(11-1)-715

Brief Title: AN INVESTIGATION OF THE ELECTRICAL AND OPTICAL PROPERTIES OF SEMICONDUCTORS AND INSULATORS WHICH HAVE BEEN IRRADIATED BY FAST NEUTRONS

Investigators: B. R. Gossick

Scope of Work

The topics under investigation in this program include the following:

(a) Disordered regions in neutron irradiated semi-conductors and insulators.
(b) The electronic properties of pile irradiated rutile.

Single crystals of sodium, barium and calcium fluoride are being irradiated with x-rays. The crystals are then examined, using a spectrophotometer to measure the optical absorption bands introduced by irradiation. The optical absorption is being studied as a function of x-ray energy and exposure. Attention is particularly directed toward the absorption band expected from plasma oscillation of electrons in colloidal metal particles formed by the print-out process.

The electrical resistivity of partially reduced n-type semiconducting rutile is being studied as a function of exposure to pile radiation, using samples with room temperature resistivity in the range 0.3 to 6 ohm-cm. The resistivity is being observed over the temperature range 250-500°K. With a dose 10^{16} neutrons/cm^2 the variation in resistivity is within a few percent, but with 10^{17} neutrons/cm^2 changes become apparent which are easily annealed. The resistivity increases with irradiation, and the percentage change is greater with low resistivity material. Studies are being directed toward determining the nature of electronic states introduced by the irradiation.

Contractor: Bartol Research Foundation of The Franklin Institute, Philadelphia, Pennsylvania

Contract: AT(30-1)-2730

Brief Title: SOLID STATE INVESTIGATIONS UTILIZING ELECTRON-BOMBARDMENT PHENOMENA

Investigators: Martin A. Pomerantz

Scope of Work

This research deals primarily with measurements of low-temperature conductivity in solids after electron irradiation. Theoretical analysis of the scattering process and investigation of Hall mobilities also will be conducted.

Proposed research contemplates utilizing the new 2-Mev electrostatic accelerator, as well as the linear accelerator which will be maintained in operating condition, and which will continue to be employed as a means of bombarding specimens for those experiments in which the measurements are conducted with separate equipment some time after high energy electron irradiation. In addition to further experiments involving MgO, studies of alkali halides, diamond and perhaps other interesting crystals would be undertaken.

Contractor: Bausch & Lomb Optical Company, Rochester, New York

Contract: AT(30-1)-1312

Brief Title: IRRADIATION DAMAGE TO GLASS

Investigators: N. J. Kreidl

Scope of Work

The absorption curves of doped fused silicas show a complex structure which is composed of several gaussian shaped bands. The characteristics of these bands (intensity, half width and energy of maximum) as obtained by the resolution of the absorption curve will help determine which bands depend mainly on the alkali and which ones are due to aluminum within the silica structure. By applying Smakula's equation, one can calculate the percentage of impurities which contribute to the formation of color centers.

The role of alkali mobility can be determined by densification and compaction of the fused silica structure attained by high pressure. Thus, examination of fused silica exposed to high pressures is expected to give valuable information on its radiation properties.

Other systems, e.g., aluminum-phosphorus and aluminum-silver impurities and application of absorption studies of other techniques, e.g., thermoluminescence, help further understanding of the silica structure. The prevention of radiation coloration by cerium will be studied in more detail.

Contractor: Brookhaven National Laboratory, Associated Universities, Inc. Upton, Long Island, New York

Contract: AT(30-2)-Gen-16

Brief Title: FUNDAMENTAL STUDY OF NEUTRON IRRADIATION ON THE PROPERTIES OF IRON AND OTHER BCC METALS

Investigators: J. G. Y. Chow, S. B. Mc Rickard, D. H. Gurinsky

Scope of Work

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 irons alloyed with an interstitial element such as carbon, a ferrite-stabilizing element such as chromium, and austenite-stabilizing elements such as nickel and manganese. Work on other bcc metals such as Mo, Ta and Nb is planned. Mechanical tests at temperatures ranging from ambient to that of liquid helium are being made on pre- and post-irradiation specimens to determine the following material parameters: yield strength, fracture strength, tensile strength, true stress-strain relationship, work hardening coefficient, tensile ductile-brittle transition, reduction in area, uniform elongation, and hardness. Similar properties will be determined on irradiated specimens thermally annealed at a series of temperatures to study the recovery of properties. Physical properties such as electrical resistivity and damping capacity are being studied. Metallographic studies and x-ray diffraction studies to determine lattice parameter changes, and electron microscopy studies are being planned to approach the problem on the atomistic scale.

Contractor: Brown University, Providence, Rhode Island

Contract: AT(30-1)-1772

Brief Title: RADIATION EFFECTS IN SOLIDS

Investigators: Rohn Truell

Scope of Work

The primary objectives of this program are to study radiation effects in solids by ultrasonic techniques. "In reactor" measurements of attenuation and velocity change are performed during irradiation (a continuation of work now underway on quartz) together with high frequency measurements before and after irradiation. Following the above measurements attenuation changes are measured during annealing and as high in temperature as the curie point (576°C). High frequency measurements are again made after annealing. Measurements on other materials such as Al_2O_3 are underway.

Included in this program is a study of the interaction between dislocations and point defects in NaCl, especially at low temperatures. An exploratory investigation of a possible influence of ultrasonic stress waves on the interaction between cold neutrons and thermal stress waves or lattice vibrations also is planned.

Contractor: Canisius College, Buffalo, New York

Contract: AT(30-1)-1810

Brief Title: INVESTIGATIONS IN IRRADIATED VITREOUS SILICA

Investigators: Herman A. Szymanski

Scope of Work

Work has been completed on the following projects:

1. Color centers in aluminium oxide induced by x-ray and cobalt 60 irradiation and bleached by ultraviolet and heat.

2. Kinetics of radiation damage in vitreous silica, analysis of the activation energy spectrum using a 650 computer.

3. Annealing of vitreous silica damaged by high pressure.

The purpose of this work was to obtain an understanding of the processes involved in radiation damage. To further achieve this the objectives for further work will be to extend the color center studies to use reflectance infrared spectroscopy as a tool. In addition work will be completed on high pressure induced damage in vitreous silica.

Contractor: (The) Franklin Institute Laboratories for Research and Development, Philadelphia, Pennsylvania

Contract: AT(30-1)-2002

Brief Title: AN EXPERIMENTAL STUDY CONCERNING THE BASIC MECHANISM OF RADIATION DAMAGE

Investigators: H. G. F. Wilsdorf and I. G. Greenfield

Scope of Work

The purpose of this investigation is to study the nature of radiation damage and radiation hardening in metals. The methods employed so far are (1) determination of the stress-strain curves for irradiated and nonirradiated single crystals; (2) the comparison of the slip line structures on the surfaces of the deformed crystals; and (3) the direct observation by a diffraction electron microscope technique of the radiation-produced defects and their interaction with glide dislocations.

The presence of prismatic dislocation loops in neutron bombarded copper has been confirmed, and the cleaning out of these prismatic loops by glide dislocations has been observed. This information together with the conclusions obtained from a study of the mechanical strength and the deformed surfaces of irradiated copper have given sufficient evidence so that a hardening mechanism could be proposed. Also, experiments with irradiated nickel and molybdenum have been continued in order to obtain more details about the mechanism of radiation damage in other metals. Annealing experiments, although not complete, have shown that prismatic loops appear in nickel and molybdenum after the proper annealing treatment. The effect of impurities on the formation of prismatic dislocation loops also is being investigated.

Contractor: General Atomic, San Diego, California

Contract:

Brief Title: IRRADIATION EFFECTS ON GAS-METAL REACTIONS

Investigators: J. Martin Tobin

Scope of Work

This research program deals with the general subject of radiation effects in metals and gas-metal reactions. The program can be divided into two phases. Phase one involves a study of the oxidation of copper during irradiation. Preliminary data using a sensitive manometric technique show that the oxidation process contains three kinetic stages. The effect of time, temperature, oxidation pressure, and neutron flux on these stages will be investigated. Data on the kinetics of oxidation will be supplemented by etch pit studies. The second phase of the proposed program entails a study of the effects of radiation on the solubility of inert gases on metals. Initial work will be performed on the rate of solution of helium in copper during irradiation.

Contractor: Michigan, University of, Ann Arbor, Michigan

Contract: AT-11-1(760)

Brief Title: QUANTITATIVE HARDNESS OF IRRADIATED AND UNIRRADIATED CRYSTALS

Investigators: R. M. Denning

Scope of Work

The principal objective of this program is the measurement of the change of hardness of diamond with respect to crystallographic direction as a result of fast neutron bombardment. Studies are also being conducted on the change of density, the ultraviolet absorption and the infrared absorption. It has been noted from the study in progress that after irradiation the hardness of the diamond is not constant throughout the crystal. It is proposed that the nature of this variation of hardness within an irradiated diamond be investigated. Incidental to the above work, electron spin resonance spectra are to be taken.

Contractor: Minnesota, University of, Minneapolis, Minnesota

Contract: AT(11-1)-532

Brief Title: EFFECTS OF ATOMIC RADIATION AND OF MOLECULAR ORIENTATION ON MECHANICAL BEHAVIOR OF LINEAR SOLID HIGH POLYMERS

Investigators: C. C. Hsiao

Scope of Work

This research involves the development of a theoretical analysis concerned with the orientation effect of a relatively general model solid. Experimental data will be obtained concurrently to determine whether the theoretical predictions are reliable. An attempt also will be made to correlate the effects of gamma irradiation and of molecular orientation on the strength of some linear polymer solids.

The general behavior of layered viscoelastic media is of great interest. Some preliminary investigations on this subject are being carried out. In addition, the much needed important time-dependent nature of fracture of some viscoelastic media as a result of pulse propagation will be sought. Efforts will also be devoted to studying mathematically the stress waves in viscoelastic solids.

Contractor: National Bureau of Standards, Washington, D.C.

Contract: NBS Project No. 1501-11-15515

Brief Title: THERMOCHEMICAL STUDY OF IRRADIATION EFFECTS

Investigators: Edward J. Prosen

Scope of Work

The objectives of this program are to develop a high-temperature calorimeter for the precise measurement of heats of solution or reaction; to make calorimetric determinations of the increase in energy content due to neutron irradiation of quartz, amorphous silica, and other crystalline and amorphous substances; and to determine heats of formation of selected compounds, such as refractories, silicates, and high temperature species.

A calorimeter presently is being built for heats of solution or reaction at elevated temperatures. The associated control equipment for automatically maintaining adiabatic conditions, for measuring temperatures with a platinum thermometer or with thermocouples, for accurate time measurements, and for accurate energy-input measurements, have been assembled and tested. Provision is being made so that later data can be taken automatically on tape, ready for input into the IBM 704 digital computer. This will greatly increase the number of data points obtained and increase the precision of the measurements. Work is now being concentrated on the actual reaction vessel.

While work on the reaction vessel and associated heater, stirrer, and thermocouples is being carried on, presently existing calorimeters will be used to measure some heats of formation of compounds of interest. It is planned to complete the calorimeter and start measurements in fiscal year 1962. The tape unit for automatic data recording will be added after manual operation has been perfected.

Contractor: Nebraska, University of, Lincoln, Nebraska

Contract: AT(11-1)-525

Brief Title: STUDIES OF IMPERFECTIONS IN SOLIDS

Investigators: Edgar A. Pearlstein

Scope of Work

Experimental work is being conducted on (1) stored energy in x-rayed alkali halide crystals, (2) radiation effects in metals (3) ionic conductivity of alkali halide crystals.

(1) For x-rayed NaCl, a graph of stored energy vs. F center concentration between 2.5 x 10^{17} and 6.4 x 10^{17} F centers/cm^3 yields a straight line with slope of about 8 ev/F center. Measurements do not extend to lower densities, but the average stored energy at 2.5 x $10^{17}/cm^3$ is about 3 e.v./F center.

(2) Measurements are being made of the increase in electrical resistivity of copper due to irradiation with protons in the energy range 50 - 350 Kev at liquid nitrogen temperature. Data so far indicates an energy dependence which might not be in agreement with theory. Also being studied is the effect of irradiating at oblique incidence, in a search for possible surface effects, and the non-linearity of damage vs. dose.

(3) It has been found that for d.c. conductivity in NaCl, the activation energy decreases as the impurity concentration increases.

An attempt is being made to detect nonlinearity of the ionic conductivity by applying a high voltage signal of two sine waves, and detecting the beat signal.

Contractor: Pennsylvania State University, University Park, Pennsylvania

Contract: AT(30-1)-2792

Brief Title: THE MECHANISMS OF FISSION GAS DIFFUSION IN GRAPHITE

Investigators: Ward S. Diethorn and Philip 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 will consist of three phases in the order listed below. Phase 1 will be the chief effort during the first year of the program.

Phase I

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 experiments the mechanisms will be used to guide the interpretation of the in-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: AT(30-1)-1858

Brief Title: EFFECT OF RADIATION ON DYNAMIC PROPERTIES OF HIGH POLYMERS

Investigators: John A. Sauer and A. E. Woodward

Scope of Work

Studies will be carried out to provide greater understanding of the effect of irradiation on polymers and to give further information concerning the relationship between physical properties of polymers and their composition and structure.

With regard to radiation effects, the studies will include: investigations of cross-linking efficiency in quenched and annealed isotactic polypropylene specimens; measurements of dynamic mechanical properties of some irradiated polymers; measurements of the temperature dependence of the proton magnetic resonance of irradiated polypropylene samples, and extension of previous experimental and theoretical work on energy disposition in polymers during reaction radiation.

Our studies on the nature and type of internal motions in polymers will also be extended. These studies will include: further NMR studies at various temperatures of different polymers and their monomers such as 3-methyl butene-1, 4-methyl pentene-1, deutered methyl methacrylate, etc; theoretical investigations of the motion of simple chemical groups and of their potential barriers to rotation; development of sensitive apparatus for dielectric and thermal expansion measurements on various polymers from $4.2^{\circ}K$ on up; NMR studies on polyethylene single crystals and of the influence of fold period and of heat treatment; theoretical and experimental studies of sound propagation in polystyrene and polythylene rods and plates; and investigations of dielectric properties of polymers in solution.

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