MASTER

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SOLID STATE PHYSICS PROGRAM

ANNUAL PROGRESS REPORT

ATOMIC ENERGY COMMISSION

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CASE WESTERN RESERVE UNIVERSITY

UNIVERSITY CIRCLE CLEVELAND, OHIO 44106

INTRODUCTION

This report describes our research activity during the period from November, 1970 through October, 1971.

Professor Schuele has requested and received a continuation of his leave of absence at Bell Telephone Laboratories, Columbus, for a second year. Dr. Carl Andeen has joined us as a Research Associate to continue this productive work with dielectric constants. Dr. George Juras has finished his post-doctoral appointment and is now at Battelle Memorial Institute.

Professional activities of the faculty, in addition to the research covered in this report, included the publication of Volume 6 of "Physics of Thin Films", edited by Professor Hoffman and M. H. Francombe. The second volume of the review journal "Critical Reviews in Solid State Sciences", edited by Professors Schuele and Hoffman, is now current. Professor Taylor's quantum solid state text is being favorably received.

Examination of Appendix I will show that three graduate students have joined our research effort and seven have received degrees. The category of Graduate Summer Students contains first-year graduate students who are supported by the University but who desire to carry out research in our area. Two NSF-supported summer undergraduate research students also contributed to our efforts.

Completed research is described in detail in Technical Reports. Seven such reports have again been issued during this past year and are listed in Appendix I. Appendix III contains the status of twenty-two papers in various stages of publication from reprints through preprints. Work that has not yet been drawn together for publication will be treated in more detail in the body of this report.

The body of this report is grouped into three areas: (A) Thin Film Physics; (B) Cohesive Properties of Crystals; and (C) Solid State Theory. Thin Film Physics is directed by Professor Hoffman. Highlights in this area include the evaluation of a technique for the rapid determination of the small grain size found in films, using the small diffracted area possible with the high-voltage electron microscope. One origin of mechanical stress in nickel films has been calculated using only the grain size as the single unadjustable parameter. Professor Schuele and Dr. Andeen's program in Cohesive Properties has given such accurate values of the dielectric constants that it is being extended to a wider frequency range. A patent using the capacitance measurement as a pressure gage is presently being filed through COO. Theoretical developments by Professor Taylor and his students include precision integrated density of states calculations for one dimensional systems and an investigation of Onsager phase factors of current importance to experimentalists.

All the faculty associated with this project have spent approximately 50% of their effort on the research described during the academic year, and 100% of their effort two summer months. With the exception of Professor Schuele, who is continuing a leave of absence started in September, 1970, they will continue to spend half of their time on this research. Professor Schuele has returned at least monthly to continue his active participation in his phase of the work.

A. Thin Film Physics

1. Torque Magnetometer Measurements - R. E. Chase and R. W. Hoffman.

The goal of this research is to grow thin, single crystal films of nickel and measure their saturation magnetization and perpendicular anistotropy by torque magnetometry in ultra-high vacuum. The films will be grown epitaxially on copper films deposited on muscovite mica.

Work during the fall consisted mainly of developing electron microscopy techniques for examining the mica and thin films. A technique of preparing mica specimens thin enough for the electron microscope was developed. Muscovite mica with a thin film of nickel deposited at room temperature was examined in the 650 keV electron microscope. The nickel films were found to be polycrystalline, as expected for the low deposition temperature. Bubble-like inclusions were observed in the muscovite similar to ones reported by other workers in the literature for phlogopite mica.

Work continued on modification of the UHV system. A six-position shutter system was designed and constructed which will allow three successive evaporations without breaking vacuum: a copper evaporation at high temperature, a copper evaporation at a lower temperature, and a nickel evaporation at the same lower temperature. Evaporating the nickel at the lower temperature minimized diffusion and evaporating copper at the same lower temperature minimizes strain from differential thermal contraction. In order to use a quartz crystal for thickness monitoring and deposition control, a commercial quartz crystal assembly was modified to provide tight damping around the crystal edges to improve thermal stability. The evaporation filament assembly was designed and built to allow successive evaporation of copper and nickel while maintaining thickness uniformity of better than 5% over the 6 cm.-long sample. Because the raw data of torque and magnetic field must be analyzed by computer and only a finite number of points are used, it was decided to eliminate the inaccuracies of retrieving the data from graph paper traces by using digital voltmeter (DVM) outputs printed on teletype. A four-plus-one digit DVM, a data coupler-multiplexer were purchased and a five-plus-one digit DVM was borrowed to allow digital readout of torque and magnetic field values. The older five-plus-one digit DVM has been modified to make its output compatible with the TTL levels of the data coupler/multiplexer. Instrumentation for this problem is now complete.

2. Mössbauer Measurements - M. N. Varma, M. Kwan and R. W. Hoffman.

The preliminary results have been published in the Journal of Applied Physics and reprints are appended. Technical Report No. 74 describes the UHV experiment in detail. The abstract reads:

TR 74 Abstract

Mössbauer spectra of thin iron films in the thickness range 1 Å to 42 Å at temperatures from 15° K to 350° K have been studied. The films are condensed and analyzed in ultra high vacuum. One observes that the films are magnetically stable when the particle size is about 90 Å at room temperature and show a transitional behavior for particle size of the order of 85 Å at room temperature corresponding to the superparamagnetic fluctuation frequency of 1.2×10^{8} radian/sec. The films having particle size of about 70 Å show a doublet spectrum at room temperature; this spectrum is interpreted in terms of superparamagnetic fluctuations and is explained as arising from magnetic hyperfine interaction and not from electric quadrupole interaction. The large separation of the doublet in the 0.4 Å film is explained in terms of an electric field gradient experienced by the iron nuclei due to the glass substrate or some contamination present on the surface of the substrate. A value of 6.7×10^{17} volts/cm^2 is estimated for the electric field gradient. Since the intensities of the two lines and the widths are nearly equal it is concluded that the sites that iron nuclei occupy are uniform and equivalent. The isomer shift of the samples is 0.17 mm/sec. and is close to that for metallic iron. The temperature dependence of the isomer shift is negative and the observed value of 4×10^{-4} mm/sec.° K is in close agreement with the value of 17 $\times 10^{-4}$ mm/sec. ° K for metallic iron determined by Hanna. Various possible explanations are included to interpret a slightly lower value of internal magnetic field compared with 33 kilogauss

for bulk iron. The variation in magnetic field from 249 kilogauss at room temperature to 298 kilogauss at 15° K for the sample of 12 Å thickness is explained in terms of superparamagnetic fluctuations. The Mössbauer lines in this sample move inwards by about 16% in changing the temperature from 350 K to 15 K, but the lines are still well resolvable and do not show the appreciable broadening that Blume's model suggest. Hence, we have concluded that Blume's theory is not adequate to explain the behavior in our films. No quadrupole splitting was detected in any of the samples thicker than 1 Å.

The spectra have been interpreted qualitatively in terms of a superparamagnetic fluctuation of the magnetization within the islands making up a film. This interpretation will be presented at the International Vacuum Congress in Boston in October and has already been accepted for publication in the conference proceedings to appear in the Journal of Vacuum Science and Technology. The abstract of this paper follows:

Mössbauer spectra for films condensed and analyzed in UHV are reported in the thickness range 1 Å to 42 Å and from 15 K to 350 K. The main features of the spectra can be explained in terms of superparamagnetic fluctuations of the magnetization within a given crystallite. Films in the thickness range 15 Å to 42 Å have a value of internal magnetic field which is slightly less than the 330 kG observed in bulk iron. As the films approach 12 Å, the hyperfine lines move inwards by about 16% when the temperature is raised from 15 K

to 350 K, but the lines are still well resolved. Assuming a simple uniaxial anisotropy model the magnetization is stable on a time scale of the Larmor period for particles > 90 Å average size and the magnetic hyperfine spectrum collapses to a doublet for particle size < 70 Å. We interpret this as arising from the complete collapse of the four excited state levels and the partial decrease of the ground state splitting corresponding to the superparamagnetic fluctuation time being limited by the frequency factor τ_0 rather than the volume or temperature. The large separation of the doublet in the 0.4 Å film is explained in terms of an electric field gradient at the iron nuclei due to the glass substrate or some contamination of the substrate.

The UHV Mössbauer system has been reworked to improve the resolution and lower the thermal losses. To this end an absorber of enriched $K_4Fe(CN)_6 \cdot 3H_2O$ in Fe^{56} has been purchased which has a narrower linewidth than the Fe^{56} in stainless steel previously employed and efforts made to minimize instrumental line broadening. To extend the low temperature capabilities of the dewar to as close to liquid helium temperatures as possible, a radiation shield has been constructed and installed that completely encloses the sample holder but opens to allow for evaporation of the film and rotation of the film to the counter. This aluminum shield is at liquid-N_2 temperature and will also serve to conserve liquid-He consumption. A new UHV dewar has been received which allows for pumping of the liquid L He cooling the sample holder. This should permit attainment of substrate temperatures below 4.2 K. Attempts are being made to discover a more efficient method of film deposition than the one presently used (resistive heating of a BN crucible containing the charge) as increased separation of the crucible and substrate necessitated by insertion of the LN_2 shield has reduced evaporating efficiency. The radiation shielding surrounding the crucible has been increased but difficulties are still being encountered in the evaporation. Different materials and methods of evaporation have been investigated but none have been feasible thus far.

3. <u>Stress Anisotrophy</u> - F. A. Doljack, M. Alexander, and R. W. Hoffman.

The work with nickel deposited in HV on [111] silicon surfaces is complete and will be submitted for publication. Technical Report No. 76, whose abstract follows, details this research.

The intrinsic stress in thin, polycrystalline nickel films vapor-deposited onto polished silicon substrates was measured by viewing the substrate deflection using an optical interference method. The method measured the force per unit width as a function of film thickness during film growth in high vacuum. The derivative of the force-per-unit-width curve gave the instantaneous stress as a function of film thickness. Runs were made at controlled substrate temperatures between -42° C and 225° C by using

a clamped-substrate geometry which provided good thermal contact to a temperature-controlled body. Films were deposited at normal incidence and at 20°, 30°, and 40° incidence. Samples were stripped from their substrates, and, since they were all approximately 2000 Å thick, a 650 KV electron microscope was used to observe directly the microstructure.

The instantaneous stress in the films was found to be constant except for the development of compressive stresses in the first 500-1000 Å of growth at the high substrate temperatures. The stresses were calculated using a grain boundary model for stress and the measured average grain sizes, which were observed to increase from about 300 Å to greater than 1000 Å over the range of substrate temperatures. The fall-off of stress with increasing substrate temperature was matched well by the calculated values, and the calculated stress values agreed within roughly 30% with the measured values. It was concluded that the constant stress was produced by a constrained grain boundary relaxation.

The compressive stresses were the result of grain boundary diffusion of silicon into the nickel film. At 200° C sufficient silicon diffuses along grain boundaries to form Ni_3Si in times less than the time of a deposition. The estimated amount of silicon that diffused was shown to be capable of producing observable compressive stresses.

The high-vacuum results just described indicate the importance of impurity atoms diffusing along the many grain boundaries in polycrystalline films. This suggests that UHV stress experiments should be carried out and we have completed a preliminary design. Several techniques used in previous work can be improved.

The problem of maintaining constant substrate temperatures during deposition may be reduced via the use of radiant heaters and a redesigned substrate clamp.

Among other thermal problems in the past has been the slight deflection of the substrate holder as the temperature is changed from room conditions to the desired deposition temperature. Previous stress measurements used a Newton's-Rings optical interference technique, which necessitated an optical flat very close to the polished substrate. After pumpdown the optical flat could not be readjusted to compensate for the deflection of the substrate. Taking data from the resulting fringes was thus often difficult. A new interferometer system has been designed using coherent laser light. This design allows a large distance between substrate and reference surface, so that adjustments may be made ex vacuo after pumpdown. A brighter fringe pattern reduces the exposure time for data photographs to 1/1000 second and thus avoids vibration difficulties.

4. Structure of Thick Films - R. Springer and R. W. Hoffman.

The average grain size is to be determined by electron microscopy. Due to the average small size of each grain (< 100 Å), conventional image techniques are not useful. The scattering of electrons at the grain boundaries, plus the inherent lack of resolution, except in unusual cases, render direct imaging techniques difficult. The root of the problem is defining the actual selected area, and distinguishing between grains by their contrast. When higher voltages are used, the image does tend to become clearer due to smaller Bragg angles.

However, it is possible, on the other hand, to look at the diffraction pattern of a small selected area. If the area is small enough, then the Debye rings become a set of discrete spots varying in intensity. Granting that these polycrystalline films have no preferred orientation, one can make calculations of the expected spot intensities.

We have carried out this analysis along these lines. Since the spin lattice interaction does not appear to play a large role, we may use Schroedinger scattering theory with the mass replaced by a relativistic electron mass, and the wavelength also corrected by a function of the energy. After the scattering intensities have been calculated, including absorption, a histogram may be anticipated by examining the number of crystallites available off the Bragg axis and the expected intensity of that deviation. Thus, knowing what maximum deviation from Bragg gives an observable reflection plus the total number of spots observed, one may deduce an average grain size.

The distribution and relative intensity of spots is obtained from a modified microphotometer. It has been altered to accept electron microscope plates and automatically analyse the "rings".

The comparison of the data from here with the "expected" data allows one to pick the maximum deviation from Bragg observed. This, along with the knowledge of the selected areas and total number of spots gives the determined grain size.

Although feasibility has been demonstrated we have not yet applied the technique.

5. Intrinsic Stress Measurement - R. Springer, J. Gasner and R. W. Hoffman.

In order to avoid thermal-expansion complications and also provide a check on the diffusion of impurities into the film from the substrate we desired to use the same material for both film and substrate. Techniques new to this Laboratory were needed to prepare metal substrates that would be mechanically stable and have an appropriate surface. The substrate is prepared by mechanically lapping the 120 μ-thick Ni to a polish with scratches and pits of only 0.1μ. A final electropolish may be used to "clean" the substrate of any imbedded lapping material.

The pumping station for this vacuum system has been completely replaced in order to provide sufficient pumping speed to maintain pressures in the 10^{-7}-Torr range during deposition of films.

6. <u>Preparation of Thick Sodium Films</u> - L. Isette and R. W. Hoffman.

As an undergraduate senior project we wished to grow thick Na films of sufficient purity and surface quality that they could be used for longitudinal magnetoresistance measurements. Although no reliable data was obtained we did develop a heated-cell geometry into which the Na could be injected in order to form hole-free films of area 1 cm^2 whose surfaces were optically good. No further work is presently contemplated.

B. COHESIVE AND DIELECTRIC PROPERTIES

1. Elastic Properties and Grüneisen Parameter of Some Semiconductors - D. Swyt and D. Schuele.

This work is now complete and is described in Technical Report No. 71. The abstract follows.

The low-temperature Grüneisen parameter, γ_L , has been determined from elasticity data for the elemental semiconductors, Si and Ge , and the semiconducting III-V compounds, GaAs, InAs and InSb. Elastic constants were measured from 300 to 4.2 K and pressure derivatives from 300 to 77 K by a conventional pulse-echo technique and show good agreement with the results of other workers. The values of γ_L calculated from the present elasticity data are systematically lower than those obtained from low-temperature thermal expansion measurements. The difference between γ_L (elastic) and γ_L (thermal) cannot be accounted for by experimental uncertainties and apparently has no basis in present theory.

2. The Elastic Properties of Copper and Copper-Nickel Alloys - J. Debesis and D. Schuele.

This work has now been completed and Technical Report No. 70 issued. The abstract follows:

The ultrasonic pulse echo technique was used to measure the elastic constants and their pressure derivatives for copper and copper-nickel alloys at temperatures of 297 K, 195 K, and 77 K. Both the elastic constants' explicit temperature dependence at fixed volume and solute concentration and the elastic constants' pure solute concentration dependence at fixed volume and temperature were determined. From these results, it was concluded that the elastic constants of the alloys can be represented by the elastic constants of pure copper plus an additive term which is only a function of solute concentration. The Debye temperature both at fixed pressure and at fixed volume was then calculated, and its dependence on solute concentration determined. The Grüneisen parameter calculated from both elastic and thermal data exhibits no significant dependence on solute concentration. The ultrasonic equation of state was then determined and compared with McQueen and Marsh's shock wave data for pure copper. Finally, a comparison of the elastic constants of the copper-nickel alloys was made with the elastic constants of the copper-zinc alloys at both fixed volume and at fixed pressure; the results for the shear constants at fixed volume were then compared with Collins' theory.

3. Continuous-Wave Measurements - D. Swyt and D. Schuele.

Continuous-wave measurements were made on some of the semiconductors with the hope of making pressure measurements at 4.2 K. The pressure transmitting system and pressure vessel with its low temperature lead thus functioned satisfactorily. However, the measurements were not reliable due to the inherent electronic leakage through and around the sample. An evaluation of the method is described in Technical Report No. 72. The abstract follows:

In an attempt to measure accurately very small changes in sound velocity with pressure, a technique which employs cw resonance was applied. The basic principle involves FM slope detection in the measurement of the changes of the mechanical resonant frequency of a composite oscillator. The effects of electrical and acoustical parameters were determined and considered in the light of other experimental and theoretical treatments. While the technique possesses extremely high resolution (.1ppm), it does not exhibit the reliability of other ultrasonic techniques in their realms of application.

4. Theory of the Static Dielectric Constant of Ionic Crystals - J. Fontanella, C. Andeen and D. Schuele.

The results of the experiments on the static dielectric constants of some alkali halides were analysed using the Clausius-Mossotti equation and the Szigeti formulation. Polarizabilities were calculated using the former and additivity studied. The Szigeti effective charge was calculated to a much higher accuracy than previous data allowed and the results were compared with the model calculations of Dick and Overhauser, Hanlon and Lawson, and Hardy. In each case, the models were found to be less accurate than implied in the literature. Finally, the results were compared with the quantum mechanical calculations of Levin and Offenbacher, Yamashita, and Mitskevich. The results of this study are contained in Tehhnical Report No. 69.

5. Theory of the Temperature and Pressure Derivatives of the Static Dielectric Constant of Ionic Crystals - J. Fontanella, C. Andeen and D. Schuele.

With the completion of the experimental determination of the temperature and pressure variation of the low frequency dielectric constant of some alkali halides, the theoretical implications of these quantities were studied. Two important results were obtained. First, the 308 K volume-independent temperature derivative of the static dielectric constant of LiF was found to be negative in disagreement with previously published results and in contrast to the positive values found for all the other measured ionic crystals of the NaCl structure. These results can be interpreted by saying that the quartic terms in the lattice potential dominate the cubic term at that temperature. There are indications that this trend may be correlated with the magnitude of the dielectric constant itself; however, further studies of medium-high dielectric constant materials are required for testing this hypothesis. The other particularly interesting result is the set of 1% upper limits for the transverse-optic-mode Grüneisen parameter, γ_{TO}, which were determined from the Szigeti formulation to be: LiF, 2.71; NaF, 2.53; NaCl, 2.83; NaBr, 2.92; KCl, 2.61; and KBr, 2.73. Unfortunately, the uncertainty associated with direct experimental values for γ_{TO} is on the order of the differences between those numbers and our upper limits; thus nothing can be said at present about the Szigeti formulation with regard to its usual interpretation.

6. The Pressure and Temperature Variation of the Low Frequency Dielectric Constant of the Alkaline Earth Fluorides - C. Andeen and J. Fontanella.

The experimental determination of the pressure and temperature variation of capacitance at room temperature for the alkaline earth fluorides has been completed. The data are presently being reduced to dielectric constant derivatives. The preliminary results indicate that the work will be particularly significant with respect to the transverse-optic-mode Grüneisen parameter as applied to the Szigeti formulation. In addition, some of the crystals have shown some interesting trace impurity effects. Much of the experimental details of these measurements is discussed in Technical Report No. 73.

7. The Low Frequency Dielectric Constants of MgO, Fused Silica, Al_2O_3, and Quartz - C. Andeen and J. Fontanella.

The 1000 Hz dielectric constant of MgO was determined to be 9.8295 and that for Al_2O_3 perpendicular to the c-axis 11.584, and that for Al_2O_3 parallel to the c-axis 9.3984. A surprising result was obtained for 5 fused silica samples obtained from General Electric Co. They showed dielectric constants from 3.8273 to 3.8287 along with a corresponding variation in loss. This nonuniformity was not expected. It was not possible to obtain an accurate value for single crystal quartz as 5 x-cuts showed a range 4.5178-4.5590, 5 y-cuts 4.5208-4.5209 and 5 z-cuts 4.6371-4.6374. The variation in the x-cuts is probably due to impurities as these crystals are natural quartz. Further work is necessary on both fused and crystalline quartz.

8. The Effects of Impurities on the Dielectric Properties of Ionic Crystals - J. Fontanella, C. Andeen and D. Schuele.

Samples of NaCl:OH and CaF_2:Eu are presently being ground and polished in preparation for measurement of their static dielectric constants and the variation of ε_s with temperature and pressure. Several orientations and concentrations are on hand for each type of crystal.

9. <u>Capacitive Pressure Gages</u> - C. Andeen, J. Fontanella and D. Schuele.

The measurement of pressure in the experiments on the pressure variation of the static dielectric constant of the alkali halides and the alkaline earth fluorides was made using the capacitive pressure gage developed in this laboratory and reported in Technical Report No. 68. This gage continues to function flawlessly and has given us the necessary increase in pressure measurement capability.

A stringent test of the instrument was made by a colleague in the department of chemistry, Dr. Scott Wellington. His experiment involved the measurement of the conductivity of liquids as a function of pressure with the time for some of the experimental runs extending to weeks. A measure of the drift and reproducibility of this instrument over this long period of being under pressure is the zero pressure readings which repeated consistently to better than 0.005 percent.

An application for patent has been filed with the Atomic Energy Commission and the paper work is proceeding under the direction of Mr. Reynolds of the Chicago Operations Office.

10. <u>Capacitance Bridges</u> - C. Andeen.

A set of three capacitance bridges has been designed to extend the high-accuracy dielectric measurements to include the frequency dependence of the static dielectric constant. This includes a

33 Hz-100 kHz-wide frequency range bridge, a 1 Hz-100 Hz low-frequency bridge and a bridge operating only at 1 kHz. These capacitance bridges, which are discussed in some detail in Technical Report No. 73, have been designed to allow highly accurate measurements of the three-terminal capacitance and dissipation factor of our samples. The two bridges covering the range from 1 Hz to 100 kHz will be used to expand the P and T measurements to determine the effects of low-level impurities and also to test for possible anomalous results in an extrapolation of a low pressure calibration of the capacitive pressure gauge to higher pressures. The 1 kHz capacitance bridge will be used in connection with the substitution method to obtain an accurate value for ε_o as a starting point in mapping ε_o versus pressure, temperature, and frequency.

The ratio transformer and divider sections of all three bridges are complete and appear quite satisfactory, and the remaining portions are sufficiently similar to a previously constructed capacitance bridge that they should not present any special problems.

C. SOLID STATE THEORY

1. Properties of Disordered Systems - P. L. Taylor, J. Gubernatis and J. Ferrante.

Our calculations during the past year have principally been directed towards a complete understanding of some special simple models of disordered systems. Particular attention has been paid to the behavior of the electronic density of states in the vicinity of band edges, as these are the crucial regions in determining the conductivity of amorphous semiconductors.

For a one-dimensional model of a disordered binary alloy we have developed a technique that allows the integrated density of states to be computed with a precision of two parts in 10^9. This allowed us to investigate deviations from the behavior predicted by Lifshitz for the way in which the density of states approaches zero at the band edge. It was found possible to show that essential singularities exist in the density of states not only at the band edges, but also at the so-called "special energies" that have been discussed by Wada for this problem. A further result of this work was the demonstration of the amount of "fine structure" in the density of states. Although it had already been shown by Borland that some fine structure existed, it had not been appreciated that a precision in which energies are measured in units of 10^{-5} of the band width would be insufficient to resolve all the structure. This has led us to conjecture that the density of states may in fact not be a differentiable function in this model; if such were to be the case it would have far-reaching implications for perturbation-theoretic treatments of similar problems. Aspects of this work have now been published [J. Phys. C: Solid St. Phys. 4, L89 (1971)].

Other work performed on the theory of disordered systems includes a continuation of our study of the transport properties of glasses, and a further pursuit of exact theorems relating to the existence of band gaps in model systems. An account of the latter work will appear in the Physical Review.

2. Effect of Magnetic Fields on Electronic States - P. L. Taylor.

The part of this work concerning the energy levels of conduction electrons in very intense magnetic fields has now been completed and has appeared in print in a paper [Phys. Rev. B3, 4091 (1971)] of which the abstract states:

From the calculation of the energy levels of conduction electrons in a simple model of a metal in a magnetic field three interesting results emerge. (a) Quantum corrections to Onsager's semiclassical quantization formula are found to be sufficiently small that the usual interpretation of the de Haas-van Alphen effect should provide an accurate measure of Fermi-surface cross sections in potassium. (b) The undetermined constant appearing in Onsager's formula is found to be 3/4 for effects due to "lens" orbits in hexagonal metals when the magnetic field lies in the basal plane. (c) The quantization of energy levels in a variety of periodic open orbits is predicted to be observable in principle through cyclotron-resonance experiments in a suitable geometry in the intermediate magnetic-breakdown regime.

This work appears to have created some considerable interest among experimentalists, as precision techniques are just now being developed that allow a measurement of Onsager phase factors in the hexagonal metals.

3. Galvanomagnetic and Size Effects in Metals - P. L. Taylor.

In these calculations our objective has remained the production of results for the galvanomagnetic properties of realistic models without the consumption of inordinate amounts of computer time. Our results for one anistropic model of a cubic metal have now appeared in print [Phys. Rev. B2, 4844 (1970)] in a paper whose abstract reads:

A solution to the linearized Boltzmann equation has been found that describes the galvanomagnetic properties of metals. The use of a vector mean-free-path function results in a solution for the conductivity tensor that is valid for any strength and orientation of the applied magnetic field. A discussion is given of the implementation of this theory to give a quantitative description of the galvanomagnetic properties of a metal when the Fermi surface and a model for the scattering of the conduction electrons are specified.

4. Band Structure Calculations Using the Relativistic KKR Method - G. E. Juras

The band structure calculations, carried out in cooperation with Professor B. Segall, have resulted in two papers. The first concerning the effective mass parameters in energy bands and the second calculating the electronic structure in zinc. The abstracts follow:

The continuation of electronic energy bands in the neighborhood of symmetry points is discussed in terms of explicit expressions derived within the Green's function method. The accuracy and convenience of these formulae is demonstrated in the calculations of specific band parameters at various symmetry points of the Brillouin zone for degenerate as well as nondegenerate states in both nonrelativistic and relativistic problems. Applications of this approach are briefly discussed.

The electronic structure of Zn has been calculated by the

Green's function method and it is found that the 3d bands lie above the conduction band minimum, not below it as previously believed. This finding is in agreement with recent X-ray emission and uv-photoemission studies. Comparison with all available experimental data shows that the calculated band structure is in good accord with the data not only in the immediate vicinity of the Fermi energy, E_F , but in the entire energy range from the bottom of the conduction band ($\sim$ 11 eV below E_F) to a few eV above E_F.

5. Mutually Orthogonal Orthogonalized Plane Waves - G. E. Juras.

This work was done in cooperation with J. E. Monahan at ANL and Professors R. Thaler and C. Shakin who are nuclear theorists at Case Western Reserve University. The preprint is appended and the abstract follows:

A basis set of mutually orthogonal OPW's is constructed. As an example of the utility of this basis set, these orthogonal OPW's are applied in the simplification of the secular equation of the one-electron problem in a periodic potential.

APPENDIX I

Personnel Associated with the Contract

<u>Professional Staff</u>

Richard W. Hoffman, Professor of Physics
Donald E. Schuele, Associate Professor of Physics (On leave)
Philip L. Taylor, Associate Professor of Physics
Carl G. Andeen, Research Associate
George E. Juras, Research Associate

<u>Research Assistants and Thesis Students</u>

P. M. Alexander
R. E. Chase
J. R. Debesis
F. A. Doljack
J. Ferrante
J. J. Fontanella
J. J. Gubernatis
C. W. Hagerling
M. Kwan
R. W. Springer
D. A. Swyt
M. N. Varma

<u>Summer Graduate Students</u>

P. Cardon

<u>Undergraduate Students</u>

L. Isett
A. Lewansky (Summer NSF)
J. Gasner (Summer NSF)

<u>Machinist</u>

J. Jaroscak

<u>Secretaries</u>

Z. M. Clifford
M. E. Young

APPENDIX II

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Technical Reports

No. 69 The Dielectric Properties of Some Alkali Halides, J. J. Fontanella COO-623-165

No. 70 The Elastic Properties of Copper and Copper-Nickel Alloys, J. R. Debesis COO-623-166

No. 71 The Grüneisen Parameter of Some Semiconductors from Elasticity Data, D. A. Swyt COO-623-167

No. 72 The Pressure Derivatives of Elastic Constants by a FM-CW Technique: An Evaluation, D. A. Swyt COO-623-168

No. 73 Accurate Determination of Dielectric Properties, C. G. Andeen COO-623-169

No. 74 UHV Mössbauer Emission Spectra in Thin Iron Films, M. N. Varma COO-623-170

No. 76 The Origins of Stress in Thin Nickel Films, F. A. Doljack COO-623-172

APPENDIX III

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Publications

The following papers were cited in reports of previous years or this current year. Reprints are now being sent under separate cover.

Pressure and Temperature Derivative of the Elastic Constants of AgCl and AgBr, K. F. Loje and D. E. Schuele, J. Phys. Chem. Solids 31, 2051 (1970) COO-623-138

Accurate Determination of the Dielectric Constant by the Method of Substitution, C. G. Andeen, J. J. Fontanella and D. E. Schuele, Rev. Sci. Inst. 41, 1573 (1970) COO-623-150

Low Frequency Dielectric Constants of LiF, NaF, NaCℓ, NaBr, KCℓ and KBr by the Method of Substitution, C. G. Andeen, J. J. Fontanella and D. E. Schuele, Phys. Rev. B2, 5068 (1970) COO-623-153

The Low Frequency Dielectric Constant of the Alkaline Earth Fluorides by the Method of Substitution, C. G. Andeen, J. J. Fontanella and D. E. Schuele, J. App. Phys. 42, 2216 (1971) COO-623-153

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Appendix IV

EQUIPMENT REPORT

AEC Contract AT(11-1)-623

Case Western Reserve University

for the period 1 February 1971 through 30 September 1971

PURCHASED TO DATE: (30 September, 1971)

ITEM	DATE PURCHASED	COST
Digital Voltmeter	30 July	$725.25

October 1971