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UNIVERSITY CIRCLE

CLEVELAND, OHIO 44106

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ABSTRACT

The present status of seven problems in thin film physics, ten in cohesive and dielectric properties, and three in solid state theory is outlined. Some especially significant results follow: Spin-wave calculations of spin-1/2 amorphous ferromagnet indicated a depletion of the high-frequency and a corresponding enhancement of the low frequency density of states, resulting in a reduction of the spontaneous magnetization and the Curie temperature. Additional progress was made in the question of the existence of band gaps in electronic states in amorphous materials. High-accuracy dielectric constant measurements were carried out for a large number of materials including MgO , Al_2O_3 , fused silica, and single crystal quartz. Many samples from different suppliers were measured and indicate that a low loss at a given temperature does not necessarily indicate high purity. The pressure and temperature derivative of the dielectric constants of the alkaline earth fluorides give agreement with the recent calculations. Modifications in the capacitive high pressure gauge are discussed. A new technique for the rapid determination of small grain sizes which utilizes a high voltage electron microscope is presented along with data for nickel films. The intrinsic stress in the same films correlates with the crystallite size and a simple interplaner potential is constructed from which the stress may be calculated.

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INTRODUCTION

This report describes the research of those faculty and students directly involved in the Solid State Physics Program supported by the Atomic Energy Commission at Case Western Reserve University during the period between November, 1971 and October, 1972.

Professor Schuele returned in July from his two-year leave of absence at Bell Telephone Laboratories, Columbus. Dr. Carl Andeen continues as Research Associate. There were no other changes in senior research people.

Our faculty also had many professional activities other than the research described in this report. We mention particularly Professor Taylor's attendance at the Institute of Physics Conference on Solid State Physics in Manchester, U.K. and invited lecture at the Eleventh Eastern Theoretical Physics Conference at the University of Connecticut as well as several colloquia. Professor Hoffman continues his second term as a Director of the American Vacuum Society. He presented lectures at the Thin Film Gordon Research Conference, and the ARPA/MRC Conference on Future Directions in Optical Surfaces and Coatings. Professors Schuele and Hoffman continue to edit "Critical Reviews in Solid State Sciences" of which the third volume is currently being published. Professor Schuele and his colleagues have experienced many interactions resulting from the accuracy of their dielectric constant measurements, and these will be discussed later.

Appendix I lists the personnel active in the program. Three graduate students have joined our research effort, while five have received degrees. All those who completed their research are presently employed, although two are in non-permanent postdoctoral positions. One undergraduate physics major also contributed to our Summer research.

Four technical reports have been issued during the year, and represent completed problems. These are listed in Appendix II. In addition twelve papers from preprint through reprint stages are detailed in Appendix III. Research that is in progress will be emphasized in the body of this report.

Three research areas are identified: (A) thin film physics; (B) cohesive and dielectric properties of crystals, and (C) solid state theory. The first area is directed by Professor Hoffman. The most significant accomplishment has been the quantitative prediction of intrinsic stress in metallic films. Impurity effects resulting from diffusion along grain boundaries have been identified, in particular for the case of nickel films condensed on various substrates. The second area, under Professor Schuele, is the precision measurements of dielectric properties; many interactions have developed between this program and other laboratories. Dr. P. Heydemann at NBS has calibrated the capacitive high pressure gage, and NBS has requested that we extend the range to 225, 000 PSI. Dr. T. Adams of Los Alamos has requested the services of Dr. Andeen as a consultant. In addition, the pressure gage has demonstrated excellent stability in use by Dr. S. Wellington on the Case Western Reserve University campus. Dr. D. Jones of the Communications Research Center of Canada, has requested that we measure the

dielectric constant of titanium silicate. The results of the continued interaction with Professor J. Fontanella, who is now at the U. S. Naval Academy, can be seen from the joint research described later. In the third area, solid state theory, new results by Professor Taylor include the calculation of the spontaneous magnetization and Curie temperature of amorphous ferromagnets and the discovery of a magnetoresistance linear in the strength of the applied magnetic field for a variety of models of simple metals.

All the faculty associated with this project have spent approximately 50% of their effort during the academic year on the research described and 100% of their effort for the two summer months.

Professor Schuele was on leave until 1 July, 1972.

A. THIN FILM PHYSICS

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

Progress in this area has been disappointingly slow. The evaporation apparatus has been modified where necessary, and installed in the UHV system. The digital print-out instrumentation has been assembled and checked out and a new data coupler/multiplexer was obtained after several fruitless returns of the original one to the factory for the correction of an intermittent malfunction. To date no data for the saturation magnetization of Ni/Cu/mica oligatomic films have been obtained.

2. Mössbauer Measurements - M. Kwan and R. W. Hoffman.

Although modifications in the servo drive and the new narrow-line absorber were carried out easily, a solution to the evaporation-source problems proved to be difficult. The resistivity-heated crucible used in our earlier studies prevented deposition on low-temperature substrates as well as being a source of contamination of the evaporant. To eliminate these problems we have developed and installed an electron beam gun that will evaporate material from milligram amounts of source charge, this is an important consideration, as our sources are radioactively doped. This electron gun utilizes the "pendant drop"

geometry whereby the tip of a thin suspended wire of the source material is bombarded by electrons from a filament below. The thermal radiation and contamination problems are avoided since (1) the source is not in contact with anything at the point of evaporation and (2) the energy for the evaporation is supplied by the high voltage between the filament and the pendant drop. As the wire is about 0.010" in diameter, a power of 2-3 watts is sufficient to deposit material at modest rates. As a result the substrates may now be held near He temperatures when films are condensed. A thermal radiation shield completely enclosing the substrate was installed last year, and this has been redesigned to be more efficient and practical.

The computer programs used for the analysis and fitting of the Mössbauer spectra have been modified and a number of additions written to provide greater versatility and efficiency.

3. Stress Anisotropy - F. A. Doljack and R. W. Hoffman.

This work was presented at the 1972 International Conference on Thin Films in Venice, and has been accepted for publication in Thin Solid Films. The abstract reads:

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. 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.

As a function of thickness, 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 higher substrate temperatures. The magnitude of the observed tension decreased from 1.5×10^{10} dynes/cm² at 0°C to 0.4×10^{10} dynes/cm² at 200°C.

The stress resulting from a constrained grain boundary relaxation was calculated from an average grain boundary potential and the experimental grain sizes. 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% of the measured values. It was concluded that the intrinsic stress was produced by this constrained grain boundary relaxation. The compressive stresses were suspected to be diffusion-induced stresses resulting from grain boundary diffusion of silicon into the nickel film.

4. UHV Intrinsic Stress Measurement -- P. M. Alexander and R. W. Hoffman.

The new Varian UHV System for this experiment was delivered in February, 1972 and the design as well as some of the construction has been completed. A bake-out system, which is entirely automatic, allows the attainment of $2-3 \times 10^{-11}$ Torr within 24 hours. The cantilever

beam geometry was chosen so that thermal effects might be minimized as well as to facilitate our thorough understanding of the small corrections to the usual bending equations for this geometry. A new technique for measuring the deflection of the cantilevered beam has shown promise of giving great precision with relative experimental ease. A straight edge is attached to the free end of the beam and positioned next to a second straight edge. A single-slit diffraction pattern then determines how much of a laser beam is passed to a photoconductive cell. The photocell signal is a sensitive function of the beam position, albeit an unknown function which must be determined a priori by calibration. The invar supporting structure, chosen to minimize the change in substrate position due to thermal expansion during deposition, has been completed together with an OFHC copper substrate clamp and heat sink which should decrease changes in substrate temperatures during deposition. The clamp has been mounted on bearings so that the substrate may be properly positioned after vacuum pumpdown and substrate heating has occurred. To date, about half of the new construction has been completed.

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

Data for the crystallite size in nickel films has been obtained over a range of substrate temperatures from ambient to 200°C. The technique, described in an Appendix in Technical Report No. 79, provides a number for the average grain diameter in columnar growth without the necessity of line profile analysis. Values obtained from nearby

portions of a film agreed well with each other and with the values that could be obtained from direct transmission microscopy. Films deposited at temperatures less than about 200°C had column diameters of about 200 Å but did not show the systematic dependence on the substrate temperature that had been anticipated. Impurity stabilization of the size may be the explanation. For temperatures above 250°C a large increase results from recrystallization.

6. Thermal and Impurity Effects in Stress Measurements - R. W. Springer and R. W. Hoffman.

This work has been completed, and a preliminary report has been accepted for publication in Jour. Vac. Sci. Tech. (C00-623-188). Final data, together with the intrinsic stress calculations and correlation with measured crystallite sizes are reported in Technical Report No. 79 whose abstract follows:

The intrinsic stress of vacuum-deposited 2000 Å nickel films was examined and correlation between the microstructure and the measured stress was found.

The cantilever-plate technique for measuring the stress using a microbalance was analyzed in detail. The bending equations were slightly revised from the former closed form approximations used in the past. Linear bending theory was shown to be adequate for the bending arising from the stressed film. The temperature problems associated

with this technique were examined and adverse effects were minimized. No bending due to thermal gradients was observed. Stress from early stages of film growth was recorded accurately for the first time.

A new technique for determining the average grain diameter was developed. High voltage electron diffraction of a small selected area produced spotty diffraction rings. A calculation relating the spots observed and the number of grains in a diffracting volume yields an average grain diameter. Agreement between grain sizes deduced from this technique and the grains observed in bright field micrographs is good. This tends to confirm columnar growth in the nickel films.

The intrinsic stress is 0.8×10^9 dynes/cm² at 35°C and decreases to zero at a temperature of about 250°C. Substrate preparation and material were found to affect the initial mechanical properties of a growing film but do not appear to alter behavior above 1000 Å. A linear stress thickness product was observed for both films deposited on nickel as well as on NiO.

A growth process is postulated, and a quantitative calculation based on this growth model was made for the stress using the bulk parameter of nickel and the measured grain size. Agreement with the measured values is good for both the nickel and NiO coated nickel substrates. The nature of the substrate material does not appear to affect the stress after 1000 Å, as no memory of the nucleation differences is apparent.

7. Adhesion of Thin Films - C. W. Hagerling and R. W. Hoffman

A prototype of the magnetic rotor-suspension apparatus has been constructed and integrated with a vacuum chamber. The suspension apparatus consists of a means of producing a voltage proportional to the rotor height and a stable servo amplifier and signal-conditioning system which drives a solenoid to support the rotor. Since the rotors involved are less than a millimeter in diameter, a sensitive method is needed to detect their height. An attempt was made to develop such a method using a radio-frequency loss principle, but this did not work well for small rotors and consequently was replaced with an optical method. Considerable attention has been placed on ensuring the reliability of the suspension system since a momentary failure amounts to complete failure of the experimental run. Thus far rotors about 0.8 mm in diameter and the same length have been suspended for periods up to 2 days with no visible hunting and good immunity to external shock.

The immediate goal is to complete the entire prototype so that the usefulness of this method of measuring thin film adhesion can be evaluated.

B. COHESIVE AND DIELECTRIC PROPERTIES

1. Theory of the Dielectric Properties of the Alkaline Earth Fluorides - C. Andeen, J. Fontanella and D. Schuele.

The analysis of the data and corresponding theoretical calculations have been completed. This work is reported in Technical Report #75 and has been published in the Physical Review B 6, 591 (1972). Besides the dielectric data, in order to calculate the temperature independent volume derivative of the Szigeti effective charge, one needs an accurate determination of the transverse optic-mode Grüneisen parameter. Two recent measurements, (J. R. Ferraro et al., J. Chem. Phys. 55, 664 (1971) and R. P. Lowndes, J. Phys. C4, 3083 (1971)) differ by a factor of two to three over the series CaF_2 to BaF_2 and hence no definitive statement can be made with respect to this theoretically important derivative. As with the alkali halides there appears to be a correlation between the dielectric constant and its volume independent temperature derivative.

The abstract of the Physical Review article follows:

The first- and second-order 308°K pressure derivatives of the low-frequency dielectric constants of CaF_2 , SrF_2 , and BaF_2 are determined to about 0.1% and 2%, respectively. The first- and second-order 308°K temperature derivatives are determined to about 0.2% and 20%. The results are used to calculate the associated volume derivatives. It is found that Srinivasan's calculation of $V(\partial\epsilon_s/\partial V)_T$ based on Axe's

shell model agrees well with experiment. The results are also used to show that in the alkaline-earth fluorides, as in the alkali halides, the question as to the sign of the temperature-independent volume derivative of the Szigeti effective charge remains open.

2. Pressure and Temperature Derivatives of the Low-Frequency Dielectric Constants of LiF, NaF, NaCl, NaBr, KCl and KBr. - John Fontanella, C. Andeen and D. Schuele.

This work is now in print [Physical Review B6, 582, (1972)]; the abstract appears below:

The first-, second-, and third-order 308°K pressure derivatives of the low-frequency dielectric constants for LiF, NaF, NaCl, NaBr, KCl, and KBr have been determined to an accuracy of about 0.2%, 2%, and 20%, respectively. In addition, the first- and second-order temperature derivatives are established at approximately the 0.2% and 20% level. The volume-independent temperature derivative of the low-frequency dielectric constant is found to be negative for LiF and positive for the remaining crystals. This trend may be understood in terms of the interaction between the acoustic and optic modes using Szigeti's formalism for anharmonic crystals as interpreted by Fuchs. The results are also used to show that the question as to the interpretation of the Szigeti effective charge remains open for the alkali halides.

3. Pressure Variation of the Low Frequency Dielectric Constant of MgO and Al_2O_3 . - C. Andeen, J. Fontanella.

The pressure variation of the low frequency dielectric constant of MgO and the dielectrically anisotropic material Al_2O_3 at room temperature are complete and the results appear as part of Technical Report #78. The first-order and second-order pressure derivatives have been calculated and the values are of the same order of magnitude as the alkali halides and alkaline earth fluorides. Complete analysis awaits the measurements on the temperature derivatives.

4. Low Frequency Dielectric Constant of Fused Silica: - C. Andeen and J. Fontanella.

The low frequency dielectric constant of many commercially available fused silicas has been measured. The samples consisted of twelve different grades (of three each) of Amersil fused silica, eight samples of Corning Code 7940 fused silica, nine samples of General Electric fused quartz and one sample of Dynasil fused silica. These results are reported in part in Technical Report #78.

This vast collection of data clearly demonstrates that a low loss at a given temperature does not necessarily indicate a high degree of purity. If the measurements are taken at a temperature above the characteristic relaxation temperature of the impurity, one still has an indication of the impurity from the measurement of the dielectric constant itself.

Part of the motivation for this vast study is in the evaluation of these materials as possible pressure sensors for the capacitive pressure gauge. Evaluation of these possible sensors will require temperature and pressure measurements.

5. Low Frequency Dielectric Constant of Single Crystal Quartz -

C. Andeen, J. Fontanella and D. E. Schuele.

Quartz is anisotropic with regard to its dielectric properties, having two dielectric constants denoted as $(\epsilon_s)_\perp$ and $(\epsilon_s)_\parallel$. The constant $(\epsilon_s)_\parallel$ corresponds to a sample whose normal to its surface is along the crystalline C-axis and $(\epsilon_s)_\perp$ corresponds to a sample whose normal is perpendicular to the C-axis. Samples with three orientations x-cut, y-cut and z-cut, were measured. The z-cut sample yields $(\epsilon_s)_\parallel$ while both x-cut and y-cut yield $(\epsilon_s)_\perp$. The z-cut samples yielded a value of $(\epsilon_s)_\parallel = 4.637_2$ and the y-cut samples an $(\epsilon_s)_\perp = 4.520_9$. The x-cut values varied from 4.518 to 4.559 and had an appreciable loss. We attribute the spread in the x-cut values to be due to impurities, though one must investigate the possible effect of crystal misorientation. A complete tabulation of the data is found in Technical Report #78.

6. The Effects of Impurities on the Dielectric Properties of Ionic Crystals - C. Andeen and J. Fontanella.

Measurements have been made on CaF_2 : Eu and NaCl : OH. Samples of CaF_2 : Eu were obtained with impurity concentrations of 0.55%, 1% and 1.26%. The results show that the dielectric constant is increased by about 1% for concentrations of Eu on the order of 1%, which implies that the Eu enters the lattice as Eu^{3+} . No conclusion can be reached about the general trend as a function of concentration as clustering may take place. Temperature and pressure measurements should clarify this.

For the NaCl : OH samples, little change is observed in the dielectric constant at room temperature. The dielectric loss tends to decrease as the OH concentration increases, contrary to what one might expect. Lower temperature measurements will be required in order to observe the effect of the OH^- ion. The complete results can be found in Technical Report #78.

7. Temperature Variation of the Pressure Variation of the Static Dielectric Constant of the Alkali Halides and Alkaline Earth Fluorides - C. Andeen, and D. Schuele.

During the past year no measurements were made on the temperature variation of the pressure variation of the static dielectric constant. In order to make measurements at different temperatures with the same

accuracy as our pressure capabilities has required an increase in accuracy of our temperature capabilities. A platinum resistance thermometer has been obtained which will be calibrated at the National Bureau of Standards. To obtain the necessary accuracy in the resistance measurement will require the construction of a ratio transformer resistance thermometer bridge. We have consulted with R. D. Cutkosky, Institute for Basic Standards, National Bureau of Standards, concerning ratio transformer bridges and a resistance bridge will be constructed partially employing their design.

8. Instrumentation for Frequency and Temperature - C. Andeen.

A 1 kHz ratio transformer capacitance bridge has been completed and successfully tested. It has been used in making all of the measurements reported in Technical Report #78 and continues to function beyond our expectations.

Work on the 1 Hz ~ 33 Hz, and 100 Hz ~ 100 kHz bridges continues along with the resistance bridge for thermometry.

9. Capacitive High Pressure Gage - C. Andeen.

The prototype capacitive pressure gage has been used routinely over the past year by Dr. Scott Wellington, a colleague in the Department of Chemistry, to measure pressures in excess of $3,500 \text{ kgm/cm}^2$ ($1 \text{ kgm/cm}^2 = 14.223 \text{ lbs/in}^2$). Initial results of this study were reported in the last Annual Progress Report and again the gage has

continued to perform flawlessly. Several crystals were used and the zero pressure readings repeated consistently to better than 0.1 kgm/cm^2 ($\sim 1 \text{ PSI}$). The ease with which this secondary pressure standard can be used by one uninitiated in the techniques of capacitance measurements is one of its salient features.

Because of the interest shown in this gage by a variety of scientists engaged in using high pressures further development has taken place. The original prototype gage required extreme temperature control ($< .001^\circ\text{C}$) of the CaF_2 capacitive sensor because of its large temperature coefficient. The present design contains two independent pressure sensors with a reference capacitor chamber also containing two independent sensors but at atmospheric pressure. To first order this should reduce the temperature effect and thus require much less stringent temperature control. The gage requires the precise measurement of the change in capacitance over a limited range. No commercial capacitance bridge is yet available for this purpose and a limited range capacitance bridge was designed and constructed for this purpose. This bridge has now been modified to simplify its use and improve its performance.

The description and details of this second-generation capacitive gage are found in Technical Report #77, the abstract follows:

In previous reports (AEC Technical Report #63 [C00-623-150],
Rev. Sci. Instr. 42, 495 [1971]) a capacitive gage for the accurate measurement of high pressures was presented. In that paper, only the

basic idea and the results of a prototype gage were given. In another report (AEC Technical Report # 73 [COO-623-169]) the details of sample preparation and a basic description of the electronics were included. In the present paper, details of the apparatus and further comments on the electronics are presented along with recent modifications which increase the practicality of such a gage.

10. Elasticity - D. E. Schuele

Three papers have now been prepared from previously reported results. The abstracts follow.

I. The Elastic Constants and Their Pressure Derivatives of Ge, Si, Ga As, InAs and InSb.

The elastic constants and their pressure derivatives for the elemental semiconductors, Si and Ge, and the III-V compounds, GaAs, InAs and InSb, have been determined by a conventional pulse echo technique. Elastic constants were measured from 300 to 4.2°K and pressure derivatives from 300 to 77°K to pressures of 30,000 psi; the results show good agreement with those of other workers at the high temperatures where some overlap in measurements occurs. The pressure dependence of the volume of each semiconductor has been evaluated according to the Murnaghan equation of state to the pressures at which phase transitions are undergone. This compressional data is essentially independent of temperature over the range of measurement, 300 to 77°K.

II. The Grüneisen Parameter of Some Semiconductors from Elasticity Data.

The low temperature Grüneisen parameter, $\bar{\gamma}_L$ (elastic), has been determined from elasticity data for the elemental semiconductors, Si and Ge, and the semiconducting III-V compounds, GaAs, InAs and InSb. The values of $\bar{\gamma}_L$ calculated from the present elasticity data are systematically lower than those obtained from low temperature thermal expansion measurements. The difference between $\bar{\gamma}_L$ and γ_L (thermal) cannot be accounted for by experimental uncertainties and apparently has no basis in present theory.

III. The Elastic Properties of Copper and Copper-Nickel Alloys.

The elastic constants and their pressure derivatives for copper and copper-nickel alloys have been measured at temperatures of 297°K, 195°K, and 77°K, using the ultrasonic pulse echo technique. 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 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 and the results for the shear constants at fixed volume were then compared with Collins' theory.

A modification, developed with Dr. Joseph Trivisonno of John Carroll University, of the standing wave resonance technique to eliminate the coherent electrical feed-through which has limited the use of its high sensitivity is now complete. This technique uses long pulses which are frequency modulated and coherently detects the pulses. This technique will have application to the measurement of pressure derivatives of the elastic constants at low temperature.

C. SOLID STATE THEORY

1. Properties of disordered systems - P.L. Taylor, J. Gubernatis, and V.C. Acharya

During the past year a number of interesting results have emerged from our work on disordered systems in computations both from exact theories and from approximation schemes. Problems studied have included amorphous ferromagnetism in three dimensions, band gaps in electronic states in amorphous materials, and the effects of correlations between neighboring sites in alloy systems.

One topic of current interest is the question of order-disorder transitions in alloy systems. It is now appreciated that for a phase transition to occur in a one-dimensional system a certain type of long-range interaction is required. In particular the Ising model requires interactions decaying no more rapidly than the inverse square of the distance if ferromagnetism is to occur. A binary alloy in which each site on a one-dimensional periodic lattice may be occupied either by an atom of type A or one of type B bears some similarity to the Ising model, in that a two-level variable exists that defines a property of each site. The addition of initially independent electrons to this system provides an effective interaction between the otherwise independent atoms, since now the total energy of the system depends on the particular configuration of atoms.

One would not, perhaps, intuitively expect to find a phase transition occurring in this system, as it seems likely that the finite range of the auto-correlation of the electron wave functions would prevent any sufficiently long-range interactions. It was thus surprising when

Foo and Amar recently presented a calculation (Phys. Rev. Letters 25, 1748) leading to an order-disorder transformation at a finite temperature. Soon afterwards, however, Plischke and Mattis (PM) studied the same alloy model by an approach which they claimed was exact, and found a free energy lower than that of Foo and Amar, and which did not exhibit a phase transition (Phys. Rev. Letters 27, 42).

We have been able to show that while PM were indeed correct in stating that the method of Foo and Amar leads to a free energy greater than the exact value, the method of PM is itself an approximation similar to the mean-field approach to ferromagnetism. High-precision calculations that we have performed within this model do not conclusively show that the PM approximation fails to predict a phase transition at finite temperatures, and thus have reopened the question of the range of the effective interaction involved. This work has been published in the Physical Review [B6, 679 (1972)].

The question of the existence of band gaps in electronic states in amorphous materials has continued to be studied. Attention was drawn in a short note [Phys. Rev. 4, 4642 (1971)] to a connection between some earlier work supported by this contract and some more recent but less specific ideas that are currently fashionable.

The problem of amorphous ferromagnetism has now finally yielded to some detailed calculations that were performed using the transformation suggested by Taylor and Wu [Phys. Rev. B2, 1752 (1970)]. With the aid of this Green-function formalism the spin-wave density of states of a spin-1/2 amorphous Heisenberg ferromagnet was calculated. The structure of the amorphous material in the model was characterized by the same

nearest-neighbor coordination and by the same density as the corresponding crystalline material. Structural disorder was represented by the changing of the orientation of the coordination of nearest neighbors from one site to another. When compared to corresponding crystalline systems, the effects of structural disorder were found to be a depletion of the high-frequency density of states of the spin waves and a corresponding enhancement of that at low frequencies. Accordingly the spontaneous magnetization and the Curie temperature of the systems were found to be reduced. This work was described at the International Symposium on Amorphous Magnetism held in August 1972 at Wayne State University, and will be reported in the published proceedings.

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

The aim of this calculation has been the determination of the phase factor σ that appears in the Onsager quantization formula

$$\tilde{A}(\epsilon) = (n + \sigma) \frac{2\pi e}{\hbar c} \vec{B}$$

which determines the area A of an allowed orbit of an electron in a metal in a magnetic field $\vec{B}$. Work performed on this problem during the past year has included the reduction of the Schrödinger equation for a suitably simple model to a product of transfer matrices. This matrix product should be reducible to a form suitable for machine computation. As it is necessary to compute the energy eigenvalues with a precision such that the numerical errors will be at most one part in 10^7 , it was decided to postpone the programming of the problem until the magnitude of certain small correction terms could be analytically shown to be negligible.

3. Transport Effects in Metals - P.L. Taylor and P. Cardon

A solution of the Boltzmann equation for the scattering of conduction electrons in anisotropic metals has continued to be approached with a combination of analytical techniques and numerical computations. The use of various group-theoretical relations provides great simplification in evaluating the magnetoresistance of a cubic metal when the magnetic field is in a direction of high symmetry; arbitrary directions of the magnetic field, however, continue to cause us problems.

The most startling result that we have found during the past year is the fact that a magnetoresistance that is linear in the strength of the applied magnetic field is predicted in a variety of models that we have studied. It had previously been believed that such effects could not emerge from a solution of the Boltzmann equation with a realistic scattering kernel, and that the experimentally observed linearity in potassium was due to strains in the samples or to more exotic effects. We are consequently attempting to repeat our calculations for a larger variety of scattering models before publishing our results.

Some attention has also continued to be given to the subject of thermoelectric power in metals and alloys. A short note on the Seebeck coefficient in ferromagnets has been accepted for publication in The Physical Review.

APPENDIX I

Personnel Associated with the Contract

Professional Staff

Richard W. Hoffman, Professor of Physics
Donald E. Schuele, Associate Professor of Physics
Philip L. Taylor, Associate Professor of Physics
Carl G. Andeen, Research Associate

Research Assistants and Thesis Students

V. C. Acharya
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APPENDIX II

Technical Reports

- No. 75 The Pressure and Temperature Derivatives of the Low Frequency Dielectric Constants of the Alkaline Earth Fluorides. C. Andeen, J. Fontanella, and D. Schuele
COO-623-180
- No. 77 A Capacitive High Pressure Gauge: Part II Apparatus and Recent Modifications. C. Andeen, J. Fontanella, and D. Schuele.
COO-623-181
- No. 78 The Dielectric Properties of Several Insulators.
C. Andeen, J. Fontanella and D. Schuele.
COO-623-182
- No. 79 Growth Effects in Thin Nickel Films. R. W. Springer.
COO-623-183

APPENDIX III

Publications

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

The Pressure and Temperature Derivative of the Low Frequency Dielectric Constants of LiF, NaF, NaCl, NaBr, KCl, and KBr, J. Fontanella, C. Andeen, and D. Schuele. Phys. Rev. B6, 582 (1972). COO-623-165

Interpretation of Mössbauer Spectra in Thin Iron Films, M. N. Varma and R. W. Hoffman. J. Vac. Sci. Tech. 9, 177 (1972). COO-623-176

Effective Mass Parameters for Electronic Energy Bands, B. Segall and G. E. Juras. Phys. Rev. B4, 3277 (1971). COO-623-177

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APPENDIX IV

EQUIPMENT REPORT

AEC Contract AT(11-1)-623

Case Western Reserve University

for the period 1 February 1972 through 30 September 1973

PURCHASED TO DATE: (30 September, 1972)

<u>ITEM</u>	<u>DATE PURCHASED</u>	<u>COST</u>
Ionization Gauge Control	24 January 1972	\$310.00
Digital Voltmeter (to be purchased October, 1972		995.00

October 1972