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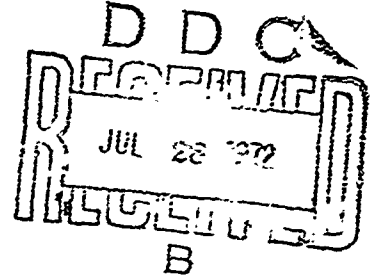
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FINAL REPORT ON GRANT #7985
Properties of Mg_2Sn

1 Feb. 1969 - 30 June 1972
R.J. KEARNEY



This is a final Technical report of the work performed under A.R.O.D. Grant #7985 - A Study of the Properties of the Semiconducting Compound Mg_2Sn . A list of published articles, and manuscripts submitted are listed in this report. Abstracts for submitted manuscripts are also enclosed.

We have been reasonably successful in our goal of investigating of the Mg_2Sn conduction band structure. As discussed in (6) we were able to identify and order the X_1 and X_3 bands and to obtain their energy shift with pressure. Data has been obtained only to 30 Kilo-bar and we have not investigated the pressure region where there is a reported phase change.

One of our initial goals was to use pressure as a tool for investigation of phonon dispersion curves. The Material Test Reactor (M.T.R.) at the National Reactor Testing Site in Idaho Falls was shut down in early 1969. Consequently our project of inelastic neutron scattering under pressure was discontinued as it was felt that too much effort would need to be expended for a successful program. Since this part of our proposal was concerned with investigation of new phenomena utilizing pressure as a tool we redirected our efforts and have performed experiments on stress induced electric fields near a metal surface. We have obtained

results on a clean $\langle 100 \rangle$ Cu surface which are reported in (7).

We have completed work concerned with the application of group theory to the lattice dynamics of Mg_2Sn (1). This complements our previous work of phonon dispersion measurements in this material.

Work on the effect of electric current on the optical properties of semiconductors, (3) and (4) have been completed.

We have also completed initial optical investigations of the compounds $\text{Mg}_2\text{Sn}_{1-x}\text{Pb}_x$. The infrared optical region from 2.5 to 50 microns was studied for x values to 0.25¹¹. In this work we observed that the transverse optic mode energy and also both the $X_1 - X_3$ electron energy separation and the $X_5 - X_1$ phonon separation changed continuously as a function of x ($x = 0.25$ was the limit of "good optical surfaces" readily attainable). Present piezo resistance experiments¹² indicate that symmetries other than (100) may be the lowest lying in the conduction band of these compounds.

Theoretical work has been completed on the effect of including spin-orbit interactions in optimized model potential calculations of lattice dynamics of simple metals¹³. Numerical calculations have been performed on Pb.

Infrared and Raman spectra has been taken on crystalline CaO ¹⁴. The interpretation of these data as regards the phonon spectra agrees well with neutron scattering data. The Lyddane-Sachs-Teller relation is found to hold for this crystal contrary to what has been reported in the literature.

In order to further explore the band structure of Mg_2Sn and related compounds we designed and constructed a wavelength modulated

optical spectrometer which is described in some detail in (9). We have taken some data on Mg_2Sn (10) and are in the process of taking data on Mg_2Sn under uniaxial stress. We feel that our spectrometer is significantly better than those described in the literature and we have a variety of experiments scheduled for our spectrometer. For example our resolution 5 Å, signal-to-noise ratio $10^5:1$ allow a variety of structure near the main E_1 peak in GaAs to be observed (9).

We have made our Mg_2Sn crystals readily available to other workers in the field. Third order elastic constant measurements and position annihilation experiments have been performed. A group at Berkeley under M.I. Cohen will test our crystals for superconductivity.

Work Performed Under AROD Grant #7985

Published Papers and Manuscripts Submitted

1. "Application of Group Theory to the Lattice Dynamics of Magnesium Sulfide," J. Phys. Chem. Solids 31, 913 (1970); R.J. Kearney, F.G. Worlton, and R.E. Schunk.
2. "Elastic Constants of SrO", J. Appl. Phys. 41, 427 (1970); D.L. Johnston, P.H. Thrasher, and R.J. Kearney.
3. "Effects of Electric Current on the Reflectivity of a Semiconductor", Phys. Rev E1, 3349 (1970); C.V. Hodge and C.A. Baumgardner.
4. "The Effect of Plasma and Hole Current on the Optical Absorption of InSb", accepted for Solid State Communications 1972; D.J. Ballegeer and C.A. Baumgardner.
- †3. "Raman Scattering in Mg_2Sn and Mg_2Si ", Solid State Comm. 9, 497 (1971); L. Laughman and L.W. Davis.
- *6. "Resistivity Pressure Dependence in Mg_2Sn ", accepted by Physica Status Solidi 1972; P.H. Thrasher and R.J. Kearney.
- *7. "Stress Dependent Contact Potential in Cu", accepted by Phys. Rev. 1972; K.H. Lenner and R.J. Kearney.
- *8. "Raman Scattering from Soft E Polaritons in $BaTiO_3$ ", accepted by Phys. Rev. 1972; L. Laughman, L.W. Davis and T. Nakamura.
9. "A 0.3 to 40 Micron Wavelength Modulation Spectrometer", submitted to Rev. Sci. Inst ; G. Hart, J. Neely, and R.J. Kearney.
10. "Wavelength Modulated Reflectivity Spectra of Mg_2Sn ", submitted to Physica Status Solidi; G. Hart and R.J. Kearney.

*Presented at the APS 1972 San Francisco meeting, Bull. of the American Physical Society 17 (1972).

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13. C.V. Hodges, "Spin Orbit Interaction in Optimized Model Potential Calculation of Lattice Dynamics of Simple Heavy Metals", Ph.D. Dissertation, University of Idaho (1971).
14. J. Hwang, "Infrared and Raman Spectra of CaO", M.S. Thesis to be submitted to the University of Idaho (1972).

Raman Scattering Line Shape of the Soft E Polariton Mode in BaTiO₃

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ABSTRACT

We report observation of Raman scattering in the polariton region by the soft E mode in tetragonal BaTiO₃. The system has excellent characteristics for testing the validity of theories that predict polariton line shapes as a function of wave number. Our spectral data are quite well fitted in the entire polariton region by a treatment recently reviewed by Barker and Loudon, in which the Nyquist theorem is applied to a simple phenomenological model of the crystal using a constant damping factor Γ . In addition, we point out that the Green's function approach by Benson and Mills yields a line shape result that here reduces to that of the Barker and Loudon model, if it is assumed the real part of the self-energy is zero and the imaginary part proportional to frequency.

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A 0.3 to 40 Micron Wavelength Modulation Spectrometer*

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ABSTRACT

A 0.3 to 40 μ wavelength-modulation spectrometer, utilizing dual beam optics and a single detector, has been designed which is free of most of the difficulties present in previously reported instruments. Over the wavelength range of the photomultiplier, this system, limited by photon shot noise is capable of an optical resolution of 6 Å. For purposes of evaluating the performance of the system, the measured derivative spectra of a holmium oxide filter and GaAs are reported.

The Effect of Plasma and Hole Current on the Optical Absorption of InSb*

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The changes in absorption coefficient due to currents flowing in p-type indium antimonide were measured. Measurements were made using polarized radiation with photon energies from .052 to .22 eV. Injecting and noninjecting samples were used with equilibrium hole concentrations of $5.4 \times 10^{15} \text{ cm}^{-3}$ at the operating temperature of 87°K. The injecting data showed several plasmon effects. The noninjecting data agreed qualitatively with the theory of Baumgardner and Woodruff.

Stress-Dependent Contact Potential in Copper

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We have measured the compressional induced change in contact potential for the (100)-face of a single crystal of copper. For a change in stress of ~ 34 atm we observed a negative contact-potential change which is interpreted as a decrease in work function. This change is -2.0 ± 1.2 $\mu\text{V}/\text{atm}$ which gives an equivalent gravitational-induced field of -1.8 ± 1.0 $\mu\text{V}/\text{M}$. The crystal face was cleaned by Ar^+ bombardment and measurements made at 2×10^{-8} Torr. Some experiments on polycrystalline copper in different environments are also reported. A simple calculation based on the Gordy equation as interpreted by Steiner and Gyftopoulos gives for a stress applied along the (001) cube axis an increase of the work function with stress of 4.3 $\mu\text{V}/\text{atm}$ for the (100) face but a decrease of 3.8 $\mu\text{V}/\text{atm}$ for the (110) face.

Pressure Dependence of Mg_2Sn Electrical Resistance*

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ABSTRACT

The electrical resistivity of single crystal Mg_2Sn is measured as a function of hydrostatic pressure to 29 kilobar at 298°K and 27 kilobar

at 320°K. Various p-type samples with varying mobilities and mobility temperature dependences are analyzed. The results for pressures less than seven kilobar may be described by a simple valence-conduction band model with an energy gap pressure dependence of $+4.75 (10)^{-6}$ eV/bar. The results for pressures up to 29 kilobar are described by a two conduction band model. The second conduction band is shown to be important even at low pressures; almost ten percent of the conduction electrons are in the upper band at room pressure and temperature. The bottom and top conduction bands are identified as X_3 and X_1 bands respectively. The energy separation between these two bands is deduced to be 0.130 eV at zero pressure. The least squares pressure coefficients of the X_3 and X_1 bands with respect to the Γ_{15} valence band are measured to be $+4.75 (10)^{-6}$ eV/bar and $-0.90(10)^{-6}$ eV/bar respectively. Estimated correction for a systematic error, introduced by the mobility dependence on pressure through the decrease of carrier lifetime when interband scattering increases, suggests that $+4.75 (10)^{-6}$ eV/bar and $-0.75 (10)^{-6}$ eV/bar may be better values for the $\Gamma_{15} - X_3$ and $\Gamma_{15} - X_1$ energy derivatives with respect to pressure. The existence of a third conduction band, with an energy location of 0.075 eV/bar with respect to the Γ_{15} band, is suggested but not definitely established by a slight upward curvature of the resistance vs pressure data below 7 kilobar.