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MAGNETO-OPTICAL OSCILLATIONS IN Cd_3As_2

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The magneto-absorption of a series of Cd_3As_2 samples with Fermi energies varying from 0.10 to 0.25 eV was measured in order to cover a larger energy interval. An excellent fit with Bodnar's model is obtained over the entire energy range, thus confirming the numerical values suggested in this model. The magnetic field however appears to flatten the Landau levels of the valence band, thus making the predicted minimum in this band unobservable.

I. Introduction and Theory

This paper reports on interband magneto-optical data taken from the transmission of identically oriented single crystals of Cd_3As_2. Similar measurements had been reported by Haidemenakis [1] but the data covered a small energy interval. Further more, Wagner [2] had analyzed these data in the light of an inverted band model and obtained a mediocre fit with an energy gap $E_o = -0.25$ eV between the conduction and light hole valence bands which is considerably different from that found by extrapolating Wagner's own magneto-optical data from $Cd_{3-x}Zn_xAs_2$ alloys ($\sim$ - 0.10 eV) or from that obtained by Bodnar (-0.095 eV) [3].

The Bodnar model is based on a Kane-type inverted band structure except that the tetragonal symmetry gives rise to a crystal field splitting and an anisotropy in the interband momentum matrix element. As a consequence, the conduction band and the heavy hole valence band are not degenerate at the Γ point as in HgTe and a surface of constant energy defines an ellipsoid of revolution whose major axis is along the crystallographic c axis. The energy E, measured from the bottom of the conduction band is related to the wavevector k by

$$\begin{aligned}\gamma(E) &= f_1(E)[k_x^2 + k_y^2] + f_2(E)k_z^2 \\ &= E(E - E_o)[E(E + \Delta) + \delta(E + 2\Delta/3)] \quad ,\end{aligned} \tag{1}$$

$$f_1(E) = P_\perp^2[E(E + 2\Delta/3) + \delta(E + \Delta/3)] \quad , \tag{2}$$

$$f_2(E) = P_\parallel^2\, E(E + 2\Delta/3) \tag{3}$$

and the z direction is taken along the c axis. E_o represents the energy gap, Δ the spin orbit coupling parameter, $P_\perp$ and $P_\parallel$ the interband momentum matrix elements respectively perpendicular and parallel to the c axis and δ the crystal field splitting parameter first introduced by Kildal [4]. By analyzing data on single crystals, Bodnar obtained the following numerical values for these band parameters: $E_o = -0.095$ eV, $P_\perp = 7.43 \times 10^{-10}$ eVm, $P_\parallel = 7.21 \times 10^{-10}$ eVm, $\Delta = 0.27$ eV, $\delta = 0.085$ eV. Figure (1) illustrates the resulting band structure for a direction relevant to our experiments.

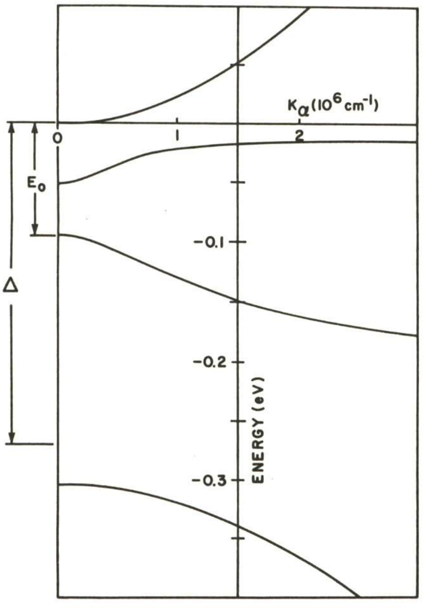

Fig. 1 Band structure near the Γ point in the k_α direction according to Bodnar's model: α is the angle between the c axis and the direction considered

It was shown by Wallace [5] that with the present model, the period P of the Shubnikov de Haas oscillations as the Landau levels pass through the Fermi level in the conduction band is given by

$$P = \frac{2e}{\hbar}\left[\frac{\sqrt{f_1(f_1\cos^2\theta + f_2\sin^2\theta)}}{\gamma}\right]_{E = E_F}, \tag{4}$$

where θ is the angle between the magnetic field and the c axis. This result can be applied to interband transitions, for a given photon energy, if E_F is replaced by the energy $E = E_C$ in the conduction band since the initial and final states of the transition do not change with magnetic field. The initial state involved in the transition is in the heavy hole band whose Landau levels in a magnetic field are located at energies $E_V(n)$ from the bottom of the conduction band where n is the quantum number. For simplicity, the energies of these Landau levels will be written

$$E_V(n) = - X - \frac{(n + \partial)\hbar eB}{m_V^*} = - X - \frac{\hbar e}{m_V^* P}, \tag{5}$$

where B is the magnetic field, ∂ the phase factor and X the energy gap between the conduction band and the heavy hole valence band whose effective mass is m_V^*. The heavy hole band in Bodnar's model is not of a standard parabolic form as implied by equation (5) but it will be seen that this is not important as far as the initial conclusions are concerned.

Finally, the photon energy $h\nu$ relates equations (4) and (5) by

$$h\nu = E_C - E_V \tag{6}$$

and the selection rule $\Delta n = 0$ applies.

II. Experimental Results and Discussion

The single crystals of Cd_3As_2 were obtained by a vapour transport method as described elsewhere [6]. Those chosen grew in the form on thin platelets with (112) faces of optical quality. Since the tetragonal unit cell of Cd_3As_2 has a c/a ratio very close to 2, one may readily show that the normal to these faces was at an angle of 54.7^o with the c axis. The magneto-transmission measurements were performed in the Faraday configuration with essentially unpolarised radiation.

The first step in analyzing magneto-oscillations is to verify the periodicity of the oscillations in 1/B and to estimate the quantum numbers. The standard plot of integers versus the inverse field at which minima in the transmission were observed gives an excellent straight line illustrating the expected periodicity but the intercept is ~ -0.8. Thus, the phase factor ∂ already included in equation (5) is not $\frac{1}{2}$ as in simple cases [7]. For sample 1B, ∂ is even found to increase smoothly with energy from +0.8 to +1.2.

A plot of $h\nu$ as a function of field is inadequate if several samples (of different ∂ and uncertain n) are to be analyzed together. A simple way to circumvent this problem is to work with the period of the oscillations, thereby eliminating the phase factor and the quantum numbers. The average periods measured for each photon energy are conveniently illustrated in Figure (2) by a plot of $h\nu$ as a function of $P^{-\frac{1}{2}}$ since in the case of cubic symmetry, such a plot yields a straight line [8].

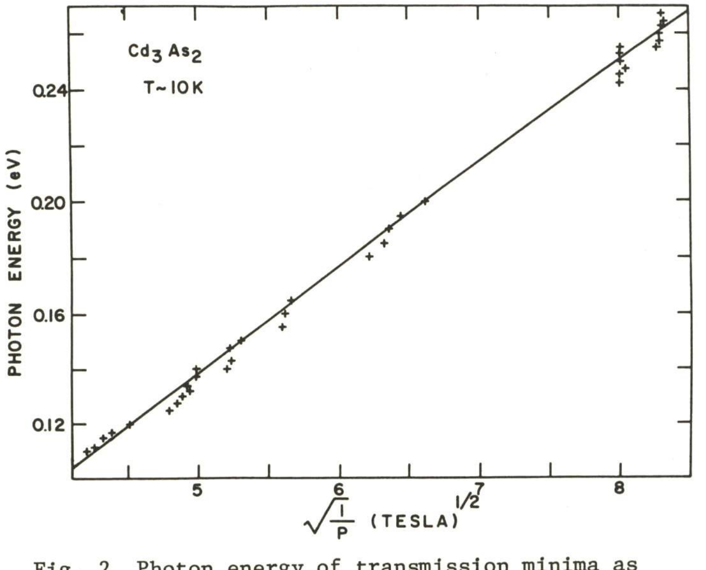

Fig. 2 Photon energy of transmission minima as a function of $P^{-\frac{1}{2}}$: The curve represents the prediction of the Bodnar model

From Bodnar's model, one may calculate the E_C (and E_V) values. This calculation first makes use of equation (4), modified for interband transitions, having inserted the numerical values found by Bodnar and a θ value of 54.7^o, as in our experiments. This gives the E_C values corresponding to the observed periods whereas the E_V values are obtained from equation (6). Surprisingly, the E_V values are virtually constant varying from 8 to 17 meV. Furthermore, most of this variation is directly related to the fine structure appearing in the data and which will be discussed below. Thus, E_V is found to be constant although the period varies by a factor of 2.5 over the investigated energy interval. This implies that the second term in equation (5) is negligible, so that $E_V \approx -X$ which regardless of the simplification postulated earlier, means that the heavy hole valence band is flat with a large effective mass in the investigated direction. This is compatible with the results of Gelten et al. [9]. The weighted average of the X_1 values is 13 meV. With this value, one can now plot $h\nu - X$ as a function on $P^{-\frac{1}{2}}$ on the same graph as the experimental points and thus obtain the curve in Figure (2). The coincidence of the experimental results to the calculated curve is quite good over the entire 0.10 to 0.20 eV range and even up to 0.25 eV, when data [10] from highly doped samples are included.

The validity of the Bodnar model and of the parameter values are thus confirmed except for the shape of the heavy hole valence band. As shown in Figure (1), a small minimum is predicted at the Γ point in an otherwise flat band. The data however do not reflect the existence of such a minimum indicating a flat band even at the Γ point. Following this result, one may question the significance of the experimental gap of $X = 13$ meV between the conduction and heavy hole bands. Since the predicted heavy hole band is flat away from the Γ point, the Landau levels would not be expected to move appreciably with a varying magnetic field. However at the Γ point, the conduction-band-like curvature would cause the Landau levels to rise with increasing magnetic fields. Thus, the Landau levels would tend to flatten out with increasing magnetic fields and remain at approximately the position occupied away from the Γ point in the absence of a magnetic field.

Finally, a consideration of the fine structure in the data is warranted. The data for a given sample usually yields a short line segment whose slope is greater than that of the general curve in Figure (2). At the highest investigated energies (> 0.20 eV), these segments are vertical, indicating the independence of the period with respect to the photon energy which is characteristic of the optical Shubnikov de Haas effect [11]. Thus, the excessive slopes of certain segments below 0.20 eV suggest that this phenomenon is still present although the main contribution is due to interband transitions. Since the optical Shubnikov de Haas effect has a period directly related to the Fermi energy and the data in our experiments were always taken near the Fermi energy of a given sample, the two effects will give almost the same period. Thus, the perturbation due to the optical Shubnikov-de Haas effect causes the fine structure in Figure (2) and also causes a variation in the phase factor referred to earlier. Also, an examination of the E_V values shows that they differ from the average value of 13 meV according to the position of the points along the line segments. Thus, most of the variation in the E_V values is due to this fine structure.

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