Magnetophonon effect in $Hg_{1-x}Cd_xTe$

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The electronic properties of the $Hg_{1-x}Cd_xTe$ ($x=0.206$) system have been investigated over a wide temperature range ($1.5<T<350$ K) using the magnetophonon effect, Shubnikov–de Haas oscillations, magnetotransmission, and Hall-effect measurements. Analysis of the data within the framework of the Pidgeon-Brown reveals the necessity for including polaron terms and a temperature-dependent interband momentum matrix element, P.

The narrow gap in systems such as $Hg_{1-x}Cd_xTe$ (HCT) implies strong interactions between the conduction and valence bands. The interactions have been included in parametrized form, in terms of the momentum matrix element P, or $E_P=2mP^2/\hbar^2$, in the Kane and Pidgeon-Brown models,[1] which are conventionally used to examine the electronic structure of these systems. The value of the momentum matrix element has been obtained by fitting to experiment assuming that this quantity is temperature independent. Our examination of the literature shows that there are experimental results which are inconsistent with this assumption and that a temperature-dependent E_P resolves these discrepancies.

In our experimental investigation of the HCT ($x=0.206\pm0.003$) system, we correlated low-temperature ($T<10$ K) Shubnikov–de Haas (SdH) and magnetotransmission measurements with the magnetophonon[2] (MP) effect over an intermediate range (50–150 K) and with high-temperature Hall measurements (77–350 K) to provide the first conclusive evidence for a temperature-dependent P in this narrow-gap system. We will emphasize the magnetophonon results partly because a wide temperature range is available and partly because anomalous results were reported in previous investigations of the temperature-dependent MP effect in this system.[3–5]

The HCT crystals used in our experimental investigation were grown at the Honeywell Electro-Optics Division. Recent observations of the metal-insulator transition and the impurity cyclotron resonance[6] in similar crystals reflect the high quality of the material. The x value was determined from room-temperature transmission Fourier transform spectroscopy measurements and the empirical formula of Hansen *et al.*[7] for the energy gap E_G. The magnetotransmission measurements were made on a 25-μm-thick sample in the Faraday configuration at $\lambda=118$ μm. Shubnikov–de Haas and magnetophonon oscillations were observed using standard field modulation techniques.

Typical Shubnikov–de Haas and magnetotransmission traces are shown in Fig. 1. The temperature dependence of the SdH peak amplitudes A, with negligible higher harmonic content, was used to obtain a value for the mass at the Fermi energy, $m_{\rm SdH}$, using conventional $\mathrm{Ln}(AH^{1/2}/T)$ versus T/H plots. A line-shape analysis of the SdH patterns with the best recursive fit[8] (BRF) was also used to measure $m_{\rm SdH}$ and determine the oscillation frequency $F_{\rm SdH}$. The results of the two techniques

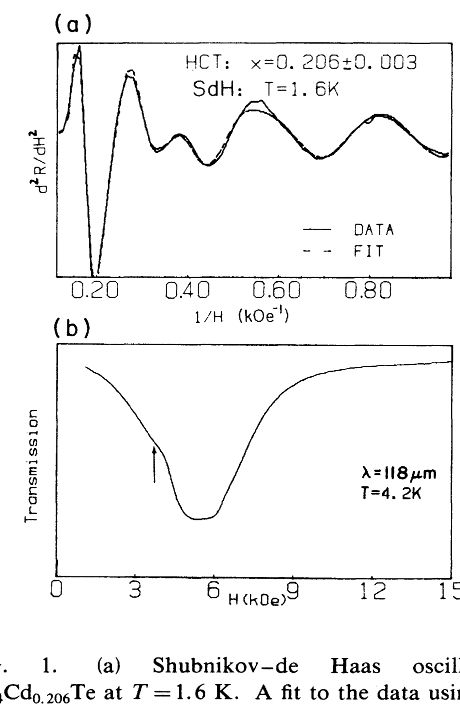

FIG. 1. (a) Shubnikov–de Haas oscillations in $Hg_{0.794}Cd_{0.206}Te$ at $T=1.6$ K. A fit to the data using the best-recursive-fit (BRF) technique is also shown. (b) Magnetotransmission in the Faraday configuration ($\lambda=118$ μm) at $T=4.2$ K. The arrow indicates combined resonance.

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were in agreement, $m_{SdH}=0.005$ $(+0.001,-0.0005)$. The frequency, $F_{SdH}=3.4$ kOe, implies a carrier density $n=1.1\times10^{15}$ cm^{-3}.

The magnetotransmission data indicate large free-carrier absorption at resonance. In addition to the cyclotron resonance peak, we observed structure at lower fields which we attribute to a combined resonance. From the transmission spectra, we estimate the effective electron g factor, $g_c\simeq170$. This value is in excellent agreement with the value determined from the spin splitting of the SdH peaks. Correlation of the magnetotransmission and SdH data allows us to directly measure the Fermi energy, $E_F\simeq9$ meV, which agrees with estimates based on the Kane model.

Our study of the MP effect in both the longitudinal (**E**||**H**) and transverse (**E**⊥**H**) configurations showed the same phase for the two effects within a factor of π. Thus in Fig. 2 we show only the transverse MP spectra for a few temperatures. There is a strong temperature dependence in the peak positions which is due in part to the large positive temperature coefficient of the gap in these materials $(dE_G/dT=3.15\times10^{-4}$ eV/K for $x=0.2$).[7] The frequency of the MP oscillation was determined with the best recursive fit and is also shown as a function of temperature in the inset of Fig. 2. The linear temperature dependence is given by $F_{MP}(T)=12+0.05T$ (kOe). The BRF also indicates the presence of a second harmonic component (Fig. 2) which increases twice as fast with temperature.

In order to determine the Landau levels associated with the SdH peaks, the cyclotron resonance, and MP oscillations, we have diagonalized the Pidgeon-Brown Hamiltonian given by Weiler.[9] To simplify calculations, we have neglected higher band contributions and warping terms so that the only nonzero parameters are E_P,

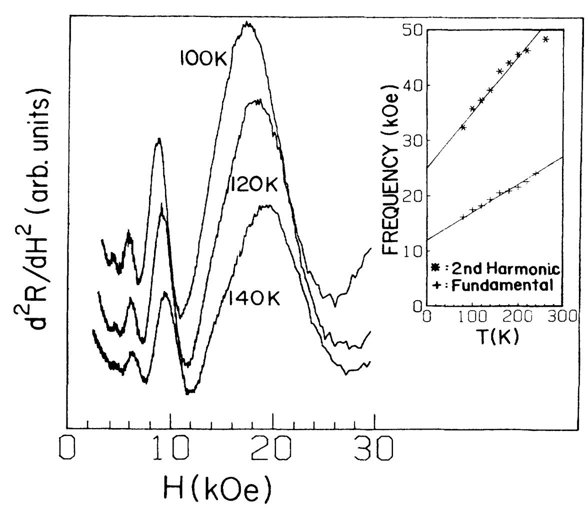

FIG. 2. The temperature-dependent transverse magnetophonon effect in HCT is shown for $T=100$, 120, and 140 K. The temperature dependence of the fundamental frequency and its second harmonic, obtained using the BRF, are shown in the inset.

E_G, and Δ. Here Δ measures the spin-orbit interaction, $\Delta\simeq1$ eV. The temperature dependence of the gap, $E_G(T)$, was determined from the expression of Hansen *et al.*[7] which has been used extensively to characterize material for device applications at Honeywell.

Raman scattering[10] and reflectivity measurements[11] have shown two types of optical phonons are present in the HCT system, one with the energy of the longitudinal-optical (LO) phonons in the pure HgTe system ($E_{LO}^{HgTe}=17.2$ meV) and another with the energy of LO phonons in the CdTe system ($E_{LO}^{CdTe}=19.6$ meV). We assume that the HgTe LO phonons are responsible for the observed MP oscillations since the sample is predominantly HgTe; i.e., the HgTe-like mode is stronger than the CdTe-like mode by a factor of 5.[12]

Attempts to fit simultaneously the low-temperature SdH, magnetotransmission, and the extrapolated zero-temperature MP frequency within the Pidgeon-Brown model were unsuccessful since the Landau-level spacing at the field given by $F_{MP}(T\simeq0)$ did not coincide with either E_{LO}^{HgTe} or E_{LO}^{CdTe}. Thus perturbative corrections to the Landau-level energies for a weak-coupling polaron ($\alpha\ll1$) in high magnetic fields ($\hbar\omega\sim E_{LO}$) were included. In terms of the Frölich (electron-phonon) coupling constant α, where

$$\alpha=(m^*/2E_{LO})^{0.5}(e^2/\hbar)[\epsilon_\infty^{-1}-\epsilon(0)^{-1}]\ , \tag{1}$$

the correction[13] is given by

$$\Delta E=\Delta E_1-\Delta E_0=-(\alpha/2)^{2/3}E_{LO}^{HgTe}\ . \tag{2}$$

Here ΔE_1 and ΔE_0 are the corrections to the energy of the $N=1$ and the $N=0$ Landau levels. Although Eq. (2) has been derived for the last MP oscillation in a parabolic band, we assume that it correctly estimates the energy corrections associated with all MP oscillations, even for a nonparabolic system.

To make the task of data fitting easier, we have used this correction factor to rescale the phonon energy, $E_{LO}^{HgTe'}=E_{LO}^{HgTe}[1+(\alpha/2)^{2/3}]=18.8$ meV, rather than correct the Landau-level energies. Our estimates [Eq. (1)] for α, $0.05<\alpha<0.07$ for $0<T<150$ K, are somewhat larger than the only previous estimate in this system ($\alpha\sim0.04$).[14] We attribute the difference to more accurate values for the static and high-frequency dielectric constants and the use of the average mass between the initial and final states rather than the band-edge mass. Rescaling the phonon energy to account for polaron effects allows us to simultaneously fit the SdH, magnetotransmission, and the MP frequency extrapolated to low temperatures, as shown in Fig. 3. In the figure, the phonon energy from the magnetotransmission experiment is used to define the energy separation of the initial and final Landau levels associated with the cyclotron and combined resonances. The corrected phonon energy, $E_{LO}^{HgTe'}$, defines the separation of the $n=0$ and the $n=1$ Landau levels at the field corresponding to the MP frequency extrapolated to low temperature, and the field values of the SdH peaks are associated with Landau levels at $E=E_F$. We have used this one-parameter (E_P) fit to determine the value of E_P at low temperatures,

$E_P(T=0)=20.5$ eV. Our result compares favorably with recent low-temperature determinations of E_P in HCT.[15,9]

Attempts to fit higher-temperature (50–150 K) MP data revealed that the MP frequency increases faster than would be expected based on the Pidgeon-Brown model with a temperature-independent E_P. Therefore we assumed that $E_P(T)=E_P(0)+\beta T$ and found that the MP data could be fit over the entire temperature range for $E_P(0)=20.5$ eV and $\beta=-0.03$ eV/K. In Fig. 3(b), we show a fit to the MP data at 100 K. Here, an integral number of Landau levels are separated by the corrected phonon energy $E_{\rm LO}^{\rm HgTe'}$ at fields given by the MP oscillation peaks.

The change in E_P with temperature probably originates from a change in the wave functions associated with the temperature-dependent gap rather than a change in the lattice constant, since experimental results show a monotonic increase of E_G with T and a nonmonotonic variation in the coefficient of linear expansion with temperature.[16] We note, however, that even the origin of the positive temperature coefficient of the gap in HCT is not understood.

Kahlert and Bauer[3] reported an anomalously large value for the temperature coefficient of the gap as a result of their study of the temperature-dependent MP effect in HCT. Using the Pidgeon-Brown model, with fixed E_P, they related the variation of the polaron mass with temperature to a variation in the gap and thus obtained a temperature coefficient for the gap which was a factor of 2 larger than the value obtained from photoconductivity[17] and optical-absorption-edge[18] studies. Use of a temperature-dependent $E_P(T)$ removes this discrepancy.

We find further support for our model in the results of Knowles and Schneider.[19] Their cyclotron resonance measurements at $\lambda=337$ μm at high temperatures (77–140 K) indicated that the cyclotron mass increases faster than the simple Kane model would predict. The Kane model with our values for $E_P(T)$ fit their data if we assume small errors in their x value (± 0.005). Thus similar behavior is observed in the magnetophonon effect and cyclotron resonance.

An examination of the literature also suggests that the values of E_P obtained by fitting high-temperature Hall-effect measurements[20] are invariably lower than values obtained from low-temperature experiments, especially if the x value is assumed known and is not treated as a fitting parameter. Therefore we have made low-field Hall measurements ($n=1/R_H e$) in the intrinsic conduction regime ($T>77$ K) to further check the self-consistency of our model. We have fitted our data by numerically solving the charge neutrality equation and have used the Kane model to obtain the density of states for the nonparabolic conduction band. The heavy-hole valence band was assumed to be parabolic. The data and fit are shown in Fig. 4. For best fit, an x value slightly larger ($x_{\rm Hall}=0.209$) than the measured value ($x=0.206$) had to be used. This difference may be due to the Burstein shift associated with carrier degeneracy at low temperatures. Thus we are able to fit the Hall data with the same $E_P(T)$ used in fitting SdH, magnetotransmission, and the magnetophonon effect. In addition, the heavy-hole mass obtained from our fit, $m_{\rm hh}^*/m=0.4$, agrees closely with the value determined from optical measurements at lower temperature.[9,12]

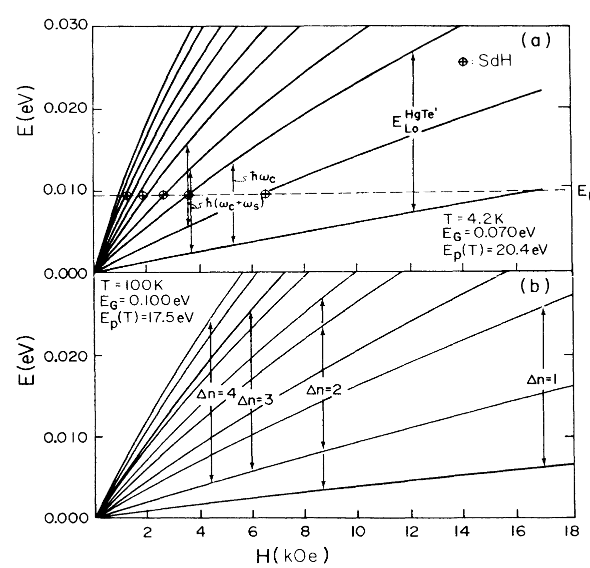

FIG. 3. (a) Shubnikov–de Haas, magnetotransmission, and the magnetophonon frequencies extrapolated to low temperature are fit to a Pidgeon-Brown calculation of the conduction band. The momentum matrix element obtained from the fit is $E_P(4.2\text{ K})=20.4$ eV. (b) A fit to the magnetophonon oscillations at $T=100$ K using the Pidgeon-Brown model. The temperature dependence of the MP frequency suggests a temperature-dependent momentum matrix element, $E_P(T)=20.5-0.03T$.

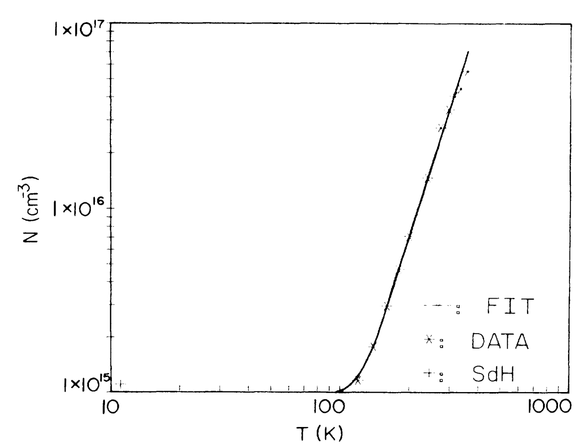

FIG. 4. The figure shows the temperature dependence of the carrier density and a fit obtained by solving the charge neutrality equation.

In conclusion, our experimental results over a wide range of temperature show that the momentum matrix element E_P is temperature dependent, $E_P(T)=20.5-0.03T$ (eV). This is an important result for systems that require the application of $\mathbf{k}\cdot\mathbf{p}$ theory since E_P and E_G are the main parameters determining the band structure. Our observations of the magnetophonon effect show the necessity for including polaron terms to successfully model data. We have also determined that the Frölich coupling constant α is somewhat larger than previously reported in the literature.

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