# Magneto-optical determination of the HgTe-CdTe superlattice band structure

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We report magnetoabsorption investigations in an $n$-type semiconducting HgTe-CdTe superlattice grown by molecular-beam epitaxy along the [111] axis. Electron cyclotron resonance and interband magneto-optical transitions are observed. The superlattice band structure is calculated with use of the envelope-function formalism along the [111] axis and in the (111) plane as well as the Landau levels when a magnetic field is applied perpendicularly to the superlattice. The interpretation of the experimental data is consistent with a small positive offset between the HgTe and CdTe valence bands.

HgTe-CdTe superlattices are new and important materials whose fundamental and technical interests are rapidly growing. They have been, for instance, proposed as a novel material for infrared detectors.[1] High-quality samples have been grown recently by molecular-beam epitaxy[2,3] and experimental studies of the electronic properties of these superlattices have been undertaken.[4–6] The band structure was calculated in the linear combination of atomic orbitals[7] (LCAO) and in the envelope-function[8] models, and an important parameter is the valence-band offset $\Lambda$ between the HgTe and CdTe valence-band edges. The common anion rule[9] predicts $\Lambda \sim 0$ in these superlattices because the energy of the valence-band edge depends essentially on the anion which is the same in HgTe and CdTe. The first experimental investigations of the electronic properties of these superlattices, using far-infrared magneto-optical techniques, concluded that $\Lambda$ is actually small and equal to about 40 meV.[4]

In this paper, we wish to present new magnetoabsorption experiments performed on a semiconducting HgTe-CdTe superlattice grown by molecular-beam epitaxy (MBE). The sample consists of one hundred periods of (100 Å) HgTe– (36 Å) CdTe grown on a CdTe(111) substrate. Intraband (cyclotron resonance) and interband magneto-optical transitions are observed and are interpreted from calculations done in the envelope-function formalism. The experimental data are actually consistent with $\Lambda \sim 40$ meV, and this positive value implies the existence of interface states[10,11] which are evanescent in both the HgTe and CdTe layers.

The sample used here was grown at 180 °C, and the interdiffusion between HgTe and CdTe is estimated to be $\sim 10$ Å for the first grown layers.[12] Although HgTe-CdTe superlattices grown by MBE present usually a $p$-type conduction at liquid-helium temperature[3] and undergo a $p$- to $n$-type transition when the temperature is increased, this sample keeps an $n$-type conduction in the whole temperature range investigated (2—300 K). The Hall mobility is found to be maximum at 77 K with $\mu_{77\,K} \sim 40\,000$ cm$^2$/V sec. Optical transmission measurements were carried out at 300 K, and the sample is found to be a semi conductor with a band gap $\sim 90$ meV, in good agreement with theoretical calculations.[13]

Before describing the experimental data, we calculate the superlattice band structure in the framework of the envelope-function approximation.[8,14] The band structures of HgTe and CdTe near the $\Gamma$ point[4] are described by the $6\times 6$ Kane Hamiltonian[14] taking into account $\Gamma_6$ and $\Gamma_8$ band edges. The interaction with the remote bands is included up to the second order by using modified Luttinger parameters, and the $\Gamma_8$ band warping is neglected by taking $\gamma_2=\gamma_3=\gamma$ (spherical approximation). The band parameters of HgTe (Ref. 15) and CdTe (Ref. 16) at 4 K used in the present calculations are listed in Table I. For a HgTe-CdTe heterostructure, a system of six differential equations for the six-component envelope function is established,[14] and the boundary conditions are obtained by writing the continuity of the wave function at the interfaces and by integrating the six coupled differential equations across an interface. This is compatible with the continuity of the probability current at the interfaces. Taking into account the superlattice periodicity, we obtain a numerical solution for the problem. Figure 1 presents the superlattice band structure calculated at 4 K for $\Lambda=40$ meV along $k_z$, where $z$ is the superlattice [111] axis, and along the momentum $k_x$ parallel to the interface [(111)

TABLE I. Band parameters of HgTe (after Ref. 15) and CdTe (after Ref. 16). $E_g$ is the interaction energy gap between the $\Gamma_6$ and $\Gamma_8$ edges, $E_p$ is related to the square of the Kane matrix element, and $\gamma_1$, $\gamma$, and $\kappa$ are the Luttinger parameters of the $\Gamma_8$ band.

| | $\gamma_1$ | $\gamma$ | $\kappa$ | $E_g$ (eV) | $E_p$ (eV) |
|---|---|---|---|---|---|
| HgTe | −15.5 | −8.9 | −10.85 | −0.302 | 18 |
| CdTe | 5.29 | 1.89 | 1.27 | 1.6 | 18 |

 

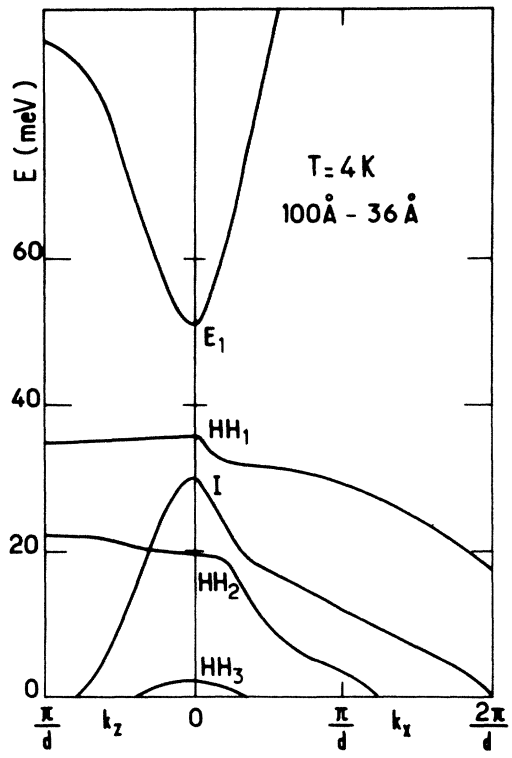


FIG. 1. Calculated band stucture along $k_z$ [111] axis and $k_x$ [in the (111) plane] of the superlattice under investigation here. The zero of energy corresponds to the CdTe valence-band edge, $d$ is the superlattice period, and $\Lambda=40$ meV.

plane]. The zero of energy corresponds to the CdTe valence-band edge while the HgTe $\Gamma_8$ band edge is located at 40 meV. The lowest conduction band $E_1$, the ground light-particle band $I$, and the heavy-hole bands $HH_1$, $HH_2$, and $HH_3$ are shown. For $k_x=0$ the light-particle and the heavy-particle bands are completely decoupled. The $I$ state lies in the forbidden energy region $(0,\Lambda)$ and corresponds to evanescent states in both kinds of layers. The envelope function is localized at the interface in such a way that $I$ is an interface state.[10,11] Such interface states are a consequence of matching bulk states belonging mainly to the light $\Gamma_8$ bands of HgTe and CdTe which display the same symmetry but opposite curvatures. The width of the $E_1$ and $I$ bands along $k_z$ is $\sim 40$ meV, and the superlattice band gap, defined as the separation between $E_1$ and $HH_1$ (the heavy-hole band) at $k=0$, is found to be 17 meV. For $k_x \neq 0$, there is a hybridization between the $I$ and heavy-hole bands which results in a complicated valence-band structure (Fig. 1). In these analyses we have assumed that the strain effects due to the small lattice mismatch between HgTe and CdTe ($\sim 0.3\%$) were negligible. The effects of strain were recently calculated by Wu and McGill[7] and by Schulman and Chang.[18] They found that strain changes the band energies only by a few milli-electron-volts. Besides, Schulman and Chang[18] have shown that the semiconducting (111) superlattice band structure is not significantly influenced by strain. In particular strains do not reverse the order of the light ($I$) and heavy hole ($HH_1$) subbands in the semiconducting (111) case, while the order is reversed in the (100) situation. In any case, the conduction band $E_1$ is nearly unaffected by strains.

To obtain the Landau-level energies, we have to calculate the band structure when a magnetic field is applied along the $k_z$ direction. The calculations are formally the same as those done at $B=0$, replacing $\mathbf{k}$ by $\mathbf{k}-(e\mathbf{A}/c)$ in the Kane Hamiltonian and taking into account the direct coupling of the electron and hole spins to the field by introducing the additional valence-band parameter $\kappa$.[19] The motion parallel to the layers is then described by a six-component vector:[20]

$$\Psi_n=(C_1\phi_{n-1},C_2\phi_{n-2},C_3\phi_n,C_4\phi_n,C_5\phi_{n-1},C_6\phi_{n+1}),$$

where $\phi_n$ is the $n$th harmonic oscillator function and $n=-1,0,1,2\ldots$. For $n\leq 1$, the coefficients $C_i$ corresponding to the negative oscillator index vanish. The calculated Landau levels associated with $E_1$, $I$, $HH_1$, and $HH_2$ are shown in Fig. 2 using $\Lambda=40$ meV. The situation is fairly complicated, and the Landau levels are strongly mixed due to the coupling between the interface state $I$ and the heavy-hole bands. The ground conduction level corresponds to $n=1$ and the second level to $n=0$.

We have performed far-infrared (FIR) magnetoabsorption experiments at 1.6 K in the Faraday configuration using a far-infrared laser (41 $\mu$m $\leq\lambda\leq$ 255 $\mu$m), carcinotrons (600 $\mu$m $\leq\lambda\leq$ 1 mm) and a $CO_2$ laser (9 $\mu$m $<\lambda<$ 11

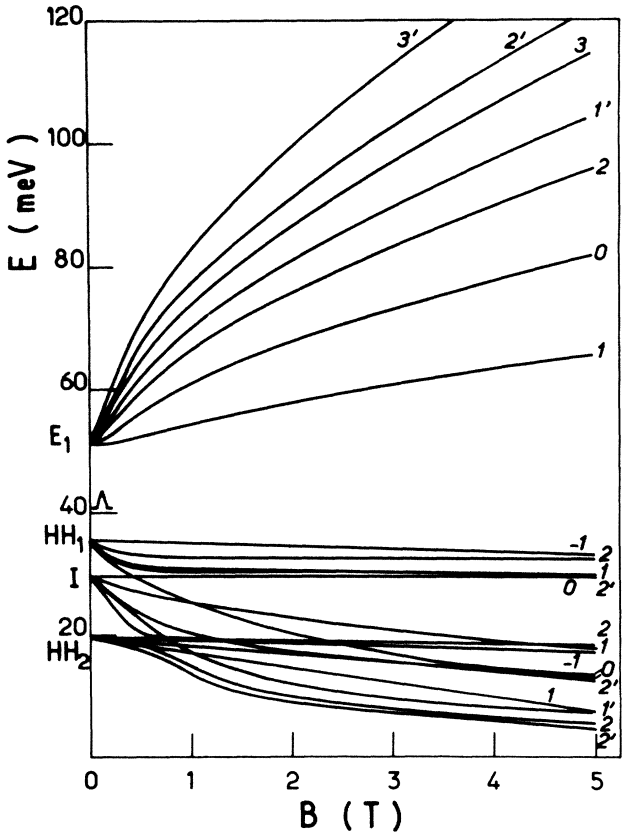


FIG. 2. Calculated Landau levels arising from the $E_1$, $I$, $HH_1$, and $HH_2$ band at 4 K. The two conduction or valence levels corresponding to the multicomponent wave function $\Psi_n$ (see text) are noted $n$ and $n'$.

$\mu$m). The magnetic field $B$ could be varied continuously between 0 and 10 T and was applied perpendicular to the plane of the superlattice layers. Figure 3(a) shows typical transmission spectra obtained for different FIR wavelengths. A single broad minimum is observed whose energy position is presented as a function of $B$ in Fig. 3(b). The transition extrapolates to an energy $\sim 0$ at $B=0$ and is attributed to cyclotron resonance arising in the $E_1$ subband. The corresponding cyclotron mass at $B \sim 1$ T is $m^*=(0.017\pm 0.003)m_0$. No transmission spectra are obtained around 20 meV which corresponds to the LO-phonon energy in CdTe and to the restrahlen band of the substrate. When the magnetic field is tilted from the normal to the layers, the line becomes broader and the minimum is shifted to a higher magnetic field because of the anisotropy of the $E_1$ conduction band (Fig. 1). The first $E_1$ intraband magneto-optical transitions, fulfilling the selection rule $\Delta n=+1$ (cyclotron resonance), corresponds to $1\rightarrow 2$ and $0\rightarrow 1'$ (Fig. 2). The dashed lines in Fig. 3(b) are the calculated energies of those two transitions using $\Lambda=40$ meV. At low photon energies ($E<15$ meV), the dashed lines correspond fairly well to the observed broad FIR absorption showing that both the $n=1$ and $n=0$ levels are populated. For $E=30$ meV, the calculated magnetic-field separation between the two lines is larger than the measured absorption. Only one transition ($1\rightarrow 2$) is observed indicating that the $n=1$ Landau level is populated at $B \sim 5$ T. It is important to point out that the interband transitions between valence and conduction Landau levels are not observable in the investigated FIR region (0—30 meV) because of the population of the ground conduction levels and of the value of the superlattice band gap. At $B=5$ T, the lowest $HH_1\rightarrow E_1$ interband transition ($-1\rightarrow 0$) would occur near 50 meV. We have no available photon energies in the range 30—100 meV, and we have studied these transitions in the $CO_2$ laser energy region (110—130 meV). Figure 4 shows that three transitions are observed for $B \geq 5$ T which extrapolate to $\sim 20$ meV at $B=0$. They are interpreted as interband $HH_1\rightarrow E_1$ transitions which obey to the selection rules $\Delta n=\pm 1$ (Faraday geometry).[20] The dashed lines in Fig. 4 represent some calculated transition energies using $\Delta n=+1$ and $\Lambda=40$ meV. Note that the experimental data could be interpreted also with transition obeying the selection rule $\Delta n=-1$ but, for the sake of simplicity, only one type of transitions is shown in Fig. 4. Such observations provide mainly information on the $E_1$ Landau levels since most of the transition energies arise from the conduction band. Precise determination of the valence Landau levels, including the effect of strains, would be obtained from FIR magneto-optical experiments in $p$-type samples, and such experiments are now in progress in our laboratory.

The results reported here are consistent with the valence-band offset $\Lambda=40$ meV previously determined from magneto-optical experiments in a semimetallic superlattice.[4] We have studied the sensitivity of the fitting procedure to the value of $\Lambda$. The superlattice band gap $E_g$ is found to decrease when $\Lambda$ increases. $\Lambda$ must be positive, otherwise charge transfer would occur between CdTe and HgTe, which is not compatible with the $p$ conduction observed in most samples at low temperature.[3] On the other hand, $E_g$ becomes less than 5 meV for $\Lambda \geq 100$ meV, and interband transitions should then be observed, in addition to cyclotron resonance, in the (0—30 meV) FIR region. The lower and upper limits for $\Lambda$ can therefore be evaluated to 0 and 100 meV, respectively, and an acceptable agreement between experiment and the calculated transitions could be obtained within these limits by taking into account the uncertainties on the sample characteristics, on the data (broad absorption minima) and on the band parameters of HgTe and CdTe used in our model. We have also investigated the interband magneto-optical transitions in a (70 Å) HgTe—(45 Å) CdTe super-

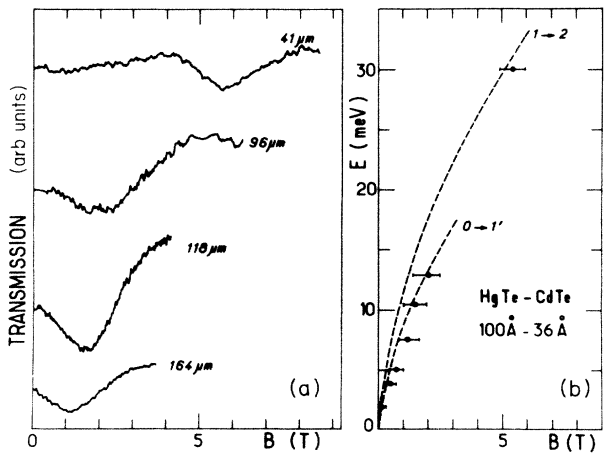


FIG. 3. (a) Typical transmission spectra obtained as a function of the magnetic field $B$ for several far-infrared wavelengths at 1.6 K. (b) Position of the transmission minima as a function of the far-infrared photon energy $E$ and the magnetic field (solid dots). The dashed lines correspond to theoretical fits of the $E_1$ cyclotron resonance.

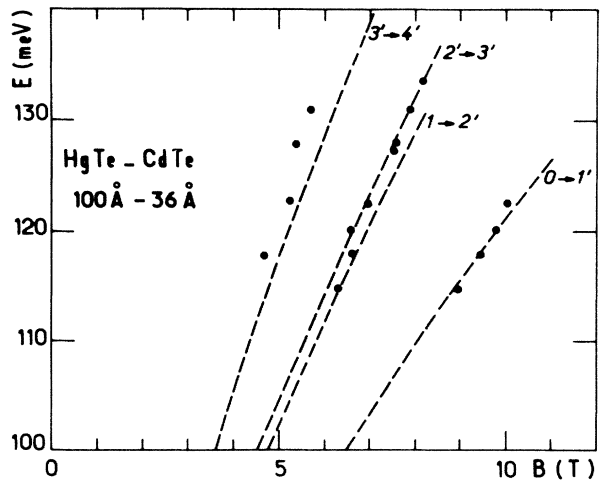


FIG. 4. Energy position of the transmission minima (solid dots) as a function of $B$ corresponding to the interband $HH_1\rightarrow E_1$ transitions observed at 1.6 K. The dashed lines correspond to the theoretical fits described in the text.

lattice. A band gap $E_g = 60 \pm 5$ meV is deduced from these experiments at 2 K and is interpreted theoretically with $\Lambda$ in the range (30—90 meV). From these investigations, one can conclude that the existence of a small positive offset ($\Lambda < 100$ meV) between the HgTe and CdTe valence bands is now strongly supported.

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