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Double hole cyclotron resonance in zero-gap HgTe-CdTe superlattices

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Magnetic-field-dependent band structures for HgTe-CdTe superlattices with zero band gap have been calculated by the transfer-matrix method. We find that there is an unusual mixing of cyclotron resonance and interband transitions. The analysis predicts that the hole cyclotron resonance should display two peaks corresponding to transitions in different regions of the Brillouin zone. Agreement with recent data showing a double peak in the Faraday geometry is quite good.

Previous investigations have demonstrated that the HgTe-CdTe superlattice band structure displays a number of interesting properties in the regime of zero energy gap.1 For example, alignment of the conduction and valence bands is indirect, the effective masses of both electrons and holes are significantly broadened (i.e., carriers with a wide range of masses coexist in the superlattice), and the hole dispersion is extremely nonparabolic. It has recently been observed that these features are manifested in the experimental free-carrier transport data.2 In the present work, we show that further effects are expected when a magnetic field is introduced. Although calculations of field-dependent band structures for HgTe-CdTe superlattices have previously appeared in the literature,3—5 there has been no discussion of the special properties which arise when the band gap is at or near zero. These properties are of particular interest because recent far-infrared magneto-optical measurements on p-type HgTe-CdTe superlattices6,7 with zero energy gap have produced features which cannot be explained by previous theories. In particular, the magnetoabsorption spectra for Faraday geometry display two peaks, both of which are allowed in the hole cyclotron resonance sense of circular polarization.

HgTe-CdTe superlattice band structures have been calculated using a transfer-matrix algorithm which has been described in detail elsewhere.8 Within the envelope function approach, an 8-band k·p model is employed rather than the 6-band approximations used by previous investigators.3,4 For zero magnetic field, the results agree well with band structures obtained by the tight-binding method.1,9 In the calculations discussed below, strain is included, a valence-band offset of 350 meV is employed, and it is assumed that the barriers contain 15% HgTe.10

Before discussing the B-dependent band structure, we briefly review the case of HgTe-CdTe superlattices in the absence of a magnetic field.2,11 If the well thickness $d_w$ is relatively narrow, the superlattice will have a positive energy gap $E_g$, i.e., for any growth-direction wave vector $k_x$, the conduction band $E_1$ will be at a higher energy than the heavy-hole band HH1 (for large valence-band offsets the light-hole-like band LH1 is well below the band edge).11 As $d_w$ is increased, $E_g$ decreases until finally $E_1$ and HH1 meet and then cross in the $k_x$ direction at some value $k_{zc}$. For $k_x < k_{zc}$, HH1 becomes the conduction band and $E_1$ the valence band. Although $E_g \approx 0$, the alignment is indirect since the conduction-band minimum is at $k_x < k_{zc}$, while the valence-band maximum is at $k_x > k_{zc}$. Electrons and holes with a wide range of masses coexist (mass broadening) because HH1 is nearly degenerate in $k_x$ and the in-plane effective mass at a given $k_x$ is proportional to the energy separation between $E_1$ and HH1, which varies significantly with $k_x$. Although $E_g \approx 0$ over the range of well widths for which $E_1$ and HH1 cross, at sufficiently large $d_w$ the entire $E_1$ band lies below HH1 and there is again an energy gap.2,12 (at $k_x \approx 0$, but not necessarily for all in-plane wave vectors).

Previous studies of HgTe-CdTe superlattices in the presence of a magnetic field along the growth direction7—5 have shown that when $E_g > 0$, the arrangement of the Landau levels is qualitatively similar to that obtained for zero-gap III-V heterostructures, such as GaAs-Ga1−xAlxAs.6,7 Both $E_1$ and HH1 are composed of two concurrent series of levels, labeled primed and unprimed, which correspond to the two 4-band sets of states discussed for bulk semiconductors by Pidgeon and Brown.13 In lowest order, magneto-optical transitions between the primed and unprimed series are forbidden. The selection rule for $\sigma^\pm$ polarization is $\Delta n = \pm 1$ for either interband or intraband (cyclotron resonance) transitions, although the two are easily distinguishable because the energy scales are much different and because interband processes go between $E_1$ and HH1 while cyclotron resonance occurs within either $E_1$ or HH1. We will see below that in the zero-gap regime, the distinction between interband and intraband processes becomes much less clear.

Figure 1 shows energy bands calculated for $d_w = 78$ Å ($N_w = 24$ monolayers), $d_h = 45$ Å ($N_h = 14$), and $B = 1$ kG. Note that the independent variable is a growth-direction wave vector, since many of the most interesting properties of the zero-gap regime originate from the strong dependence of the bands on $k_x$. The bands labeled 0 and $-2'$ represent ground-state Landau levels for $E_1$ and HH1, respectively, and their dependences on $k_x$ are quite similar to those in the absence of a magnetic field. The crossing at $k_{zc} \approx 0.13\pi/d$ separates the region in which...
perature is zero and that the Fermi level is at $-16$ meV, i.e., just below the 0 level at $k_z = 0$ and between the $-2'$ and $-1'$ (lower) levels at $k_z = \pi/d$. There will be a large number of possible interband transitions of the type $-1'$ (lower) $\rightarrow 0'$ (upper), $0'$ (lower) $\rightarrow -1'$ (upper), etc., which satisfy the $\Delta n = \pm 1$ selection rule. However, there are only two allowed processes coupling a full initial state and an empty final state which have energy differences in the range accessed by the far-infrared magneto-optical experiments of interest, i.e., less than $\approx 14$ meV: $1$ (lower) $\rightarrow 0$ and $-1'$ (lower) $\rightarrow -2'$. Note that both of these transitions have $\Delta E$ which vary considerably with $k_z$, i.e., neither will be associated with a single, sharply defined resonance. Instead, there will be a continuous spectrum of transition energies which correspond directly to the mass-broadening effect discussed previously in connection with zero-field band structures. Assuming that scattering does not cause too much additional broadening (i.e., $\omega_\tau > 1$), the maxima of the spectrum will occur near those extremal regions for which $\Delta E$ changes most slowly with $k_z$. (The situation is somewhat similar for interband transitions in InAs-GaSb superlattices.) An examination of Fig. 1 shows that there are primarily two such regions in the present example, namely those which have been labeled HCR. Although there is also a third possibility: interbandlike transitions of the type $-1'$ (lower) $\rightarrow -2'$ at small $k_z$, Fig. 1 shows that the curvature of $\Delta E(k_z)$ is greater in that case. We will find below that this process does not necessarily lead to a separate absorption peak.

In order to demonstrate explicitly that multiple maxima should occur, we now perform a simple magnetotransmission spectrum calculation for input parameters appropriate for the example discussed in the previous paragraph. Use of the Drude form for the frequency-dependent conductivity reveals that the power absorbed is approximately

$$P(\omega) = \frac{1}{2} |\epsilon|^2 \frac{\sigma_0}{1 + (\omega \tau - \omega_\tau)^2},$$

(1)

where $\epsilon$ is the optical electric field, $\sigma_0 = e^2 \tau / m_e$ is the zero-frequency conductivity, $\tau$ is the momentum relaxation time, $m_e = eB / \omega_0$ is the in-plane effective mass, and $\omega$ is the optical frequency. The cyclotron frequency may be obtained directly from Fig. 1 by equating $\hbar \omega_c$ to $\Delta E$, the energy difference between Landau levels involved in a given transition. The hole density is

$$p = \frac{eB}{2\pi^2 \hbar} \sum n \int_0^{\pi/d} dk_z f_0,$$

(2)

where $f_0$ is the Fermi distribution function and the summation is over hole Landau levels. Substituting for $\sigma_0$ in Eq. (1), we obtain

$$P(\omega) \sim \int_0^{\pi/d} \frac{\omega_c \tau dk_z}{1 + (\omega \tau - \omega_\tau)^2},$$

(3)

where for simplicity we assume that only the highest-hole Landau level is occupied. Numerical evaluation of this expression leads to the transmission spectrum shown in Fig. 2. A relaxation time of 1 ps was employed, which is
just slightly greater than the value 0.3 ps estimated experimentally by Perez et al. We see that there are in fact two absorption peaks, corresponding to the two HCR transitions indicated in Fig. 1. The peak energies of 2.0 and 5.8 meV are slightly larger than the extremal (zone boundary) values for $\Delta E$: 1.5 and 5.1 meV. Since $\Delta E$ for both transitions increase as one moves away from the zone boundaries, it should not be surprising that the “averaged” values are higher than the extremal values. On the other hand, the interband process $-1' (\text{lower}) \rightarrow 2' (\text{small } k_z)$, which was discussed in the previous paragraph, is not resolvable as a separate peak. Instead, it is part of the high-energy tail of the 5.8-meV peak.

Although our analysis is somewhat simplified since we have not incorporated overlap integrals or accounted in detail for the initial and final-state occupation statistical factors, we can nonetheless perform a first-order estimate of the magnetoabsorption peak energies. These will then be compared with the recent experimental results of Perez et al., who studied a $p$-type HgTe-CdTe superlattice with nominal well and barrier widths of 23 and 14 monolayers ($\pm 2$ monolayers). Because the band-structure calculation predicts a small positive energy gap (3 meV) for these parameters, we have increased the well width by 1 monolayer to make the superlattice semimetallic.

As in the theoretical spectrum shown in Fig. 2, the Faraday-geometry data yielded two absorption peaks, which are both allowed for circular polarization in the hole cyclotron resonance sense (in the experiment, $h\omega$ is held fixed and one finds the peak in magnetic field). In Fig. 3, the experimental results for transition energies versus magnetic field are compared with calculated values based on the zone-boundary energy differences. The theoretical curves are seen to quite accurately reproduce the main features of the data, including the nonparabolicity. It should be remembered that the only adjusted parameter in the calculation was an increase in the well width by 1 monolayer. Furthermore, we saw above that the extremal resonance energies underestimate the expected peak values, so a more detailed calculation may improve the agreement between theory and experiment.

While Perez et al. had identified the higher-energy transition as hole cyclotron resonance, the lower-energy line was previously unexplained. Spin resonance was suggested because the variation with magnetic-field angle appeared to link this line to a Voigt-geometry resonance with $\epsilon \perp \mathbf{B}$ selection (whereas the higher-energy line was linked to a Voigt resonance with $\epsilon \parallel \mathbf{B}$ selection, as generally holds for cyclotron resonance in bulk semiconductors). In a small-gap semiconductor, one expects the spin splitting to be comparable to the Landau splitting. For the band structure shown in Fig. 1, the lowest-order spin resonance transition is $-1'$ (lower at small $k_z$, upper at large $k_z$) $\rightarrow 0$. Since the two $-1'$ bands are in close proximity to the 1 bands, the $\Delta E$ for spin resonance is quite similar to the hole cyclotron resonance energy at small $k_z$ and the electron cyclotron resonance energy at large $k_z$. Therefore, if the sample is $p$ type one expects the spin resonance (which may be weak since the process is forbidden in lowest order) to be much closer to the higher energy rather than the lower energy of the two experimentally observed peaks. Although the present theory appears to account for both of the lines seen in Faraday geometry (both are interpreted as hole cyclotron resonance), the reason for the observed Voigt-geometry selection rules remains unclear. The present band-structure calculations have not yet been generalized to account for arbitrary magnetic-field direction.

Summarizing, we have presented the first theoretical study of the influence of a magnetic field on the band structure of HgTe-CdTe superlattices with zero energy gap. As in the absence of a magnetic field, the dependence on growth-direction wave vector is found to be crucial. While the ground-state Landau levels are similar to the bands at $B = 0$, the excited levels change from $E_1$ to
HH1 character (or vice versa) as $k_z$ is varied. This leads to a mixing of interband and intraband (cyclotron resonance) transitions. The variety of possible magneto-optical transitions is quite large, and the transition energies span a continuous range. However, it is explicitly demonstrated that magnetoabsorption peaks should occur near the energy differences for extremal transitions at the zone boundaries, where $AE$ does not change rapidly with $k_z$. For $p$-type samples it is predicted that there should be double cyclotron resonance peaks, one associated with transitions near $k_z = 0$ and the other with transitions near $k_z = \pi/d$. The dependences of both peak energies on magnetic field are found to be in good agreement with the experimental results of Perez et al. We are thus able to account for the previously unexplained lower-energy peak.

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10. Justification for these input assumptions is discussed in detail in Ref. 2.
14. This rule may be affected by the generality of the set of basis functions employed.
17. If $\tau = 0.3$ ps is employed, the 5.8-meV peak in Fig. 2 is still sharp, but the 2.0-meV feature ceases to have a resolvable peak. The experimental estimate for $\tau$ may have been low since it was based on the assumption that the entire linewidth is due to scattering rather than mass broadening.
18. The corresponding theoretical curves for $N_w = 23$ rather than 24 are quite similar to those shown in Fig. 3, except that both resonance energies are lower by 10–30%. If $N_w$ is increased above 24, the higher-energy resonance moves down somewhat while the lower-energy resonance moves up in energy. Beyond this, the statistical occupation factors can be affected considerably as $N_w$ is varied.