RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 32, NUMBER 8 15 OCTOBER 1985

Interface states and subbands in HgTe-CdTe heterostructures

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(Received 3 May 1985)

If one component of a semiconductor heterojunction has an inverted band gap relative to the other component, e.g., as in HgTe-CdTe, an interface state may exist depending on the valence-band offset. In a quantum well, the mixing of these interface states with the topmost heavy-hole subbands at finite in-plane wave vector changes drastically the in-plane dispersion of the heavy-hole subbands and, hence, the fundamental band gap.

There has been growing interest in the superlattices of the II-VI compounds, HgTe and CdTe, since Schulman and McGill[1] suggested that they would be promising candidates for infrared detectors. Unlike CdTe and III-V compounds, HgTe is a zero-gap semiconductor.[2] Zero-point energies of the electrons and holes in HgTe sandwiched between CdTe layers would yield a small subband gap, which can be controlled by the HgTe layer thickness. The existence of this small gap is the key to the possibility of an infrared detector.

However, the existence of an interface state[3,4] at the CdTe/HgTe interface complicates the simple picture above. In Ref. 3, the existence of the interface state was deduced only for a zero-momentum component along the interface and, therefore, no conclusions could be drawn on the possible change of the subband structure due to the interface state. In this Rapid Communication, we report our investigation into the subband dispersion for finite in-plane momentum in a quantum well in the presence of the interface states. The subband from the interface states, having an electronlike in-plane dispersion, crosses some of the heavy-hole subbands and hybridizes with them. The existence of the hybridized interface subband changes the occupation of the bands and, hence, the fundamental gap. It has an important effect on transport and the interpretation of the optical transitions.

In CdTe, the Γ_6 conduction bands lie above the Γ_8 valence bands. In HgTe, the Γ_8 bands lie above the Γ_6 bands. The fourfold set of Γ_8 bands are split into two electronlike bands and two heavy-hole bands degenerate at Γ yielding the zero gap. The Γ_6-Γ_8 energy differences in CdTe and HgTe are, respectively, 1600 and -300 meV. The value of the valence-band offset Λ is not precisely known at the present time. By the common anion rule,[1] it should be much smaller than the fundamental gaps. Analysis of magneto-optic data by Guldner *et al.*[5] indicates that Λ is positive and about 40 meV. Their analysis did not take into account the nature of the interface states and might, therefore, not be accurate. With that reservation, we take their value of Λ in our numerical estimates.

Owing to the smallness of Λ, the electronic properties of the heterostructures are mainly determined by the electronic structure at the Γ_8 band edges. As a leading-order approximation, we neglect the Γ_6 bands. The Γ_8 bands of HgTe and CdTe are adequately described by the 4×4 Luttinger Hamiltonian[6] (in atomic units) using the basis set with quantum number m_J ranging from $\frac{3}{2}$ to $-\frac{3}{2}$:

$$H(\mathbf{k}_{\parallel},k_z)=\begin{pmatrix} P+Q & -S & R & 0 \\ -S^* & P-Q & 0 & R \\ R^* & 0 & P-Q & S \\ 0 & R^* & S^* & P+Q \end{pmatrix}, \tag{1}$$

where

$$\begin{aligned} P &= E_v-\tfrac{1}{2}(k_z\gamma_1k_z+\gamma_1k_{\parallel}^2)\ , \\ Q &= k_z\gamma_2k_z-\tfrac{1}{2}\gamma_2k_{\parallel}^2\ , \\ R &= \frac{\sqrt{3}}{2}\bar{\gamma}k_-^2-\frac{\sqrt{3}}{2}\mu k_+^2\ , \\ S &= -\frac{\sqrt{3}}{2}k_-(k_z\gamma_3+\gamma_3k_z)\ , \\ k_{\pm} &= k_x\pm ik_y\ , \\ k_{\parallel}^2 &= k_x^2+k_y^2\ , \\ \bar{\gamma} &= \tfrac{1}{2}(\gamma_2+\gamma_3)\ , \end{aligned} \tag{2}$$

and

$$\mu=\tfrac{1}{2}(\gamma_3-\gamma_2)\ .$$

In the heterostructures, we choose the z axis to be normal to the interface. Within the effective-mass approximation, k_z in Eq. (1) stands for the operator $(1/i)\partial/\partial z$. The momentum parallel to the interface $\mathbf{k}_{\parallel}=(k_x,k_y,0)$ is a good quantum number in the absence of external magnetic field. The band edge E_v and the Luttinger parameters γ_1, γ_2, and γ_3 are considered as functions of z and do not commute with k_z. In Eq. (2), we have symmetrized the noncommuting products in a particular manner to preserve the Kramers doublets. This procedure is not unique but reasonable. If an extra potential $V(z)$ exists in the heterostructure, it is added to the diagonal elements of the Hamiltonian. For simplicity, in the subsequent study of the band dispersion, we neglect the band warping (setting $\mu=0$) and the linear k terms due to the lack of symmetry between the group-II and -VI atoms. The band parameters used in the present considerations are listed in Table I.

We now apply Eqs. (1) and (2) to study the electronic structure of the HgTe-CdTe heterostructures. We consider

TABLE I. Band parameters of HgTe and CdTe.

	E_v (meV)	γ_1	$\bar{\gamma}$	m_l^*	m_h^*
HgTe	0	−12.8[a]	−8.3[a]	0.034	−0.263
CdTe	−40[b]	5.3[c]	1.85[c]	−0.111	−0.526

[a]Reference 2, p. 229, and references therein.
[b]Reference 5.
[c]R. Sooryakumar, M. Cardona, and J. C. Merle, Solid State Commun. **48**, 581 (1982), and references therein.

separately the cases of zero and nonzero $\mathbf{k}_\parallel$ under the flat-band condition, i.e., $V(z)=0$. The Hamiltonian H_{ij} becomes diagonal for $\mathbf{k}_\parallel=0$. In this case, the light-particle ($m_J=\pm\frac{1}{2}$) and the heavy-hole ($m_J=\pm\frac{3}{2}$) bands are completely decoupled. The system is described by two independent Hamiltonians with a spatially varying mass [$m_l^*(z)$ or $m_h^*(z)$]:

$$H_{l,h}=-\frac{1}{2}\frac{\partial}{\partial z}[m_{l,h}^*(z)]^{-1}\frac{\partial}{\partial z}+E_v(z) \ , \tag{3}$$

where $m_l^*=-(\gamma_1+2\gamma_2)^{-1}$ and $m_h^*=-(\gamma_1-2\gamma_2)^{-1}$. Charge and current conservation lead the boundary conditions which require that $\Psi(z)$ and $(1/m_{l,h}^*)\Psi(z)$ be continuous at the interface.[7,8]

Consider the HgTe-CdTe heterojunction. Let the ideal interface be located at the plane $z=0$, with HgTe occupying the region $z<0$ and CdTe the region $z>0$. For the light particle, there is a forbidden energy region, $-\Lambda<E<0$ ($\Lambda>0$). An electronic state with energy inside the gap must be evanescent in nature. The envelope function is localized at the interface and decays exponentially in both directions $\pm z$. The derivatives at the interface have opposite signs. Such a wave function can satisfy the boundary conditions because the effective mass of the light particle $m_l^*(z)$ changes sign at the interface due to the band reversal between HgTe and CdTe. From Eq. (3), it is easy then to determine the energy eigenvalue of the interface state:

$$E_l=-\frac{m\Lambda}{m+m'}\simeq -9.4 \text{ meV} \ , \tag{4}$$

where $m=m_l^*$ in HgTe and $m'=-m_l^*$ in CdTe. The corresponding decay length for the envelope function is 110 Å in HgTe and 33 Å in CdTe. This long decay length justifies the use of the effective-mass approximation and shows the distinct nature of these interface states as compared to that of the usual short-ranged dangling bonds. It is also clear that there exists no such interface state in III-V heterostructures without the band reversal of one component. The energy of the interface state lies inside the heavy-hole continuum of HgTe. For $\mathbf{k}_\parallel\neq 0$, the interface state interacts with the heavy-hole band, and becomes a resonance level. The existence of these resonance levels will take electrons from the heavy-hole bands of HgTe, yielding an accumulation layer of heavy holes and interface electrons. Such charge rearrangement will give rise to an electrostatic interface potential and bend the bands.

We now consider the CdTe-HgTe-CdTe quantum well. Let HgTe occupy the region $-d/2<z<d/2$. As far as the interface states at $\mathbf{k}_\parallel=0$ are concerned, the quantum well can be considered as two heterojunctions in series. For a finite well width d, the interface state at left interacts with the one at right, and the energy levels split. The resulting eigenstates are symmetric and antisymmetric with respect to $z=0$:

$$\Psi_{\pm 1/2}^{(+)}(z)=\begin{cases} A\cosh(Kz), & |z|<\frac{d}{2} \ , \\ Be^{-K'|z|}, & |z|>\frac{d}{2} \ , \end{cases} \tag{5}$$

and

$$\Psi_{\pm 1/2}^{(-)}(z)=\begin{cases} C\sinh(Kz), & |z|<\frac{d}{2} \ , \\ D\,\mathrm{sgn}(z)e^{-K'|z|}, & |z|>\frac{d}{2} \ , \end{cases} \tag{6}$$

where K and K' are imaginary wave vectors in HgTe and CdTe, respectively. From Eq. (3) and the boundary conditions, the energy-eigenvalue equations are given by

$$\frac{K}{m}\tanh\left(K\frac{d}{2}\right)=\frac{K'}{m'} \text{ (symmetric)} \ , \tag{7a}$$

$$\frac{K}{m}\coth\left(K\frac{d}{2}\right)=\frac{K'}{m'} \text{ (antisymmetric)} \ , \tag{7b}$$

$$E=-\frac{1}{2m}K^2=\frac{1}{2m'}K'^2-\Lambda \ . \tag{8}$$

To determine the bulklike bound states ($E>0$) of the light particle, we replace K by ik in Eqs. (5)–(8). The envelope function inside the HgTe well becomes either the cosine or sine wave. The symmetric interface state exists for any well width d. For $d<d_c=(2m'/m^2\Lambda)^{1/2}\approx 190$ Å, Eq. (7b) has no solution, hence the antisymmetric evanescent-wave state ceases to exist. By examining Eq. (7b) and its counterpart of the real k, we find that the antisymmetric evanescent wave evolves continuously to the sine wave, when d is reduced below d_c. At this point, the envelope function in the well changes its curvature. We have solved numerically Eqs. (7) and (8) and the corresponding equations for the bulklike bound states. The resulting energies as functions of the well width are shown as solid curves in Fig. 1. As d decreases from infinity, the energy of the symmetric interface state decreases, while those of the excited states increase. Increase in the energy splitting between the symmetric interface state and the antisymmetric state is expected. We note in passing that all the bound states in the system, including the interface states, can be classified by the number of nodes in their wave functions. Similar calculations were also carried out for the heavy-hole bands which, at $\mathbf{k}_\parallel=\mathbf{0}$, are decoupled from the interface states. The results are shown as dashed curves in Fig. 1. Thus, we obtain a complete energy-level scheme for the case of $\mathbf{k}_\parallel=\mathbf{0}$.

In the case of $\mathbf{k}_\parallel\neq\mathbf{0}$, a mini-$\mathbf{k}\cdot\mathbf{p}$ method is used to calculate the subband dispersion.[9] The bound states, including light-particle and heavy-hole states, found for the case $\mathbf{k}_\parallel=\mathbf{0}$, are taken as the basis set. For a given $\mathbf{k}_\parallel$, the envelope function is expanded as a linear combination of the basis set. From Eq. (1), the energy expectation value is determined. The variational calculation immediately leads to a set of the eigenvalue equations. Solutions of the eigenvalue matrix then give the subband structure. In Fig. 2, we show the subband structure of the quantum well at $d=100$ Å. For $\mathbf{k}_\parallel=\mathbf{0}$, there are two heavy-hole and two light-particle bound states within the energy range of interest.

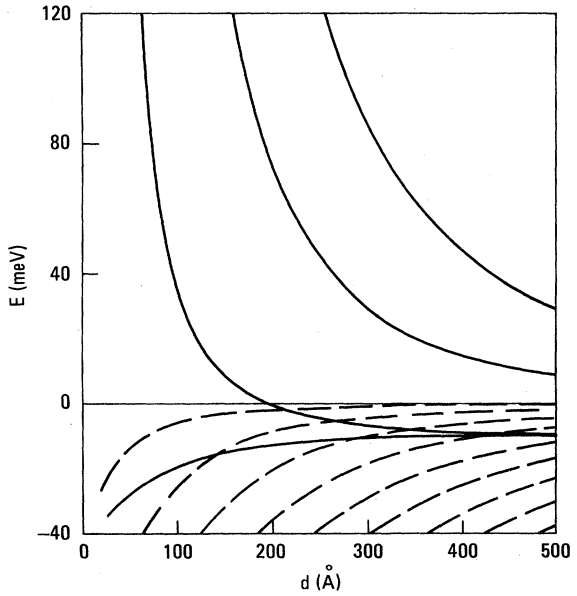

FIG. 1. The energy of $\mathbf{k}_{\parallel}=0$ states vs the well width d, in the CdTe-HgTe-CdTe quantum well. (Solid curves represent the light particle; dashed curves represent the heavy-hole bound states.)

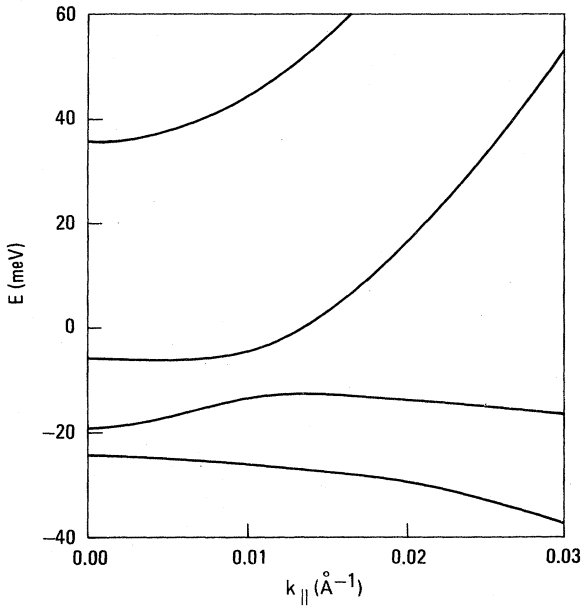

FIG. 2. The subband dispersion as a function of $\mathbf{k}_{\parallel}$ in the CdTe-HgTe-CdTe quantum well of well width $d=100$ Å.

When $\mathbf{k}_{\parallel}\neq\mathbf{0}$, the off-diagonal terms in Eq. (1) provide coupling between them. The subbands associated with the first excited states of the light particle and the heavy hole maintain, to a large extent, their original electronlike and holelike character, respectively. On the other hand, the symmetric interface state and the ground state of the heavy hole interact strongly and form two hybridized subbands. The hybridization process is easily visualized. The interface state is of the light-particle character. The corresponding subband in the quantum well has an electronlike dispersion for small $k_{\parallel}$. As $k_{\parallel}$ increases, the subband would have intercepted the one associated with the ground state of the heavy hole if there were no off-diagonal coupling. Were the interface state not there, the highest occupied level would have been on the subband edge associated with the heavy hole. The band gap of the system would then have been determined by the bulklike valence- and conduction-subband edges. In the presence of the interface state such a picture is no longer correct. For the particular quantum well ($d=100$ Å) we have considered, the lower hybridized subband is occupied by electrons, and the higher one is empty. The band gap is the hybridization gap which is about 8.5 meV. Thus, the existence of the interface states has profound effects on the electronic properties of the HgTe-CdTe heterostructures.

In summary, we have established an effective-mass theory to deal with the electronic structure of the HgTe-CdTe heterostructures. Within the theoretical framework, the nature of the interface states and their interaction with the heavy-hole bands are examined in some detail. Calculations of the electronic structure in the presence of external magnetic field, based upon an extension of this work, are currently in progress. Finally, we would like to emphasize that the existence of the interface states and the associated hybridized subband structures is new and unique in the study of heterostructures. Direct experimental verification of their existence is certainly of great interest.

One of us (Y.R.L.L.) would like to thank Dr. L. Senbetu for introducing him to the subject and Dr. D. A. Broido for useful discussions pertaining to Ref. 9. We are also indebted to Dr. H. Ikezi for his comments on the manuscript.

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