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# Effects of quasi-interface states in HgTe-CdTe superlattices

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It is shown that a new type of quasi-interface state which is an admixture of CdTe light-hole and HgTe conduction-band states exists in HgTe-CdTe superlattices near the top of the valence band. This interface state contributes significantly to optical properties.

Because HgTe is a zero band-gap material, superlattices made from alternating layers of HgTe and CdTe offer promise as being useful infrared optical materials.[1] Experimental studies of these superlattices have recently been reported[2-4] and scientific interest is rapidly growing. The first theoretical investigation of the electronic structures of HgTe-CdTe superlattices was performed by Schulman and McGill[1] within the tight-binding framework. The envelope function approach to the problem was later applied[5] and energy spectra of HgTe-CdTe superlattices with a wide range of layer thickness were predicted. Recently, calculations on optical properties of HgTe-CdTe superlattices have been reported[6] and it has been shown that the band-edge optical absorption in the HgTe-CdTe superlattice is comparable or even larger than that in the HgCdTe alloy.

In this paper we report the existence of a quasi-interface state in HgTe-CdTe superlattices, if the valence-band offset is assumed to be positive, i.e., the HgTe valence-band maximum lies above that of CdTe. Experimentally, the valence-band offset has preliminarily been determined to be 40 meV.[3] The quasi-interface state is a consequence of matching up of bulk states belonging to the conduction band in HgTe and the light-hole valence band in CdTe. Such a matching is only favorable when the bulk states to be connected are made of atomic orbitals of the same symmetry type and the effective masses on either side of the interface have the opposite sign, as is the case in HgTe-CdTe superlattices.

We demonstrate the existence of such quasi-interface states by first considering a single-interface HgTe-CdTe heterostructure in a one-band model. The model contains a positive-mass conduction band in HgTe and a negative-mass light-hole valence band in CdTe. The energy gap of the heterostructure is denoted by $V_p$ which is the same as the HgTe-CdTe valence-band offset. By imposing the boundary condition that both the wave function and the current density are continuous at the interface, one obtains a solution with energy

$$E_0 = -\frac{m_A}{m_A + |m_B|} V_p \ , \tag{1}$$

where $m_A$ and $m_B$ are the HgTe conduction-band and CdTe valence-band effective masses, respectively, and the energy zero is chosen to be at the HgTe conduction-band minimum. Since the energy $E$ falls inside the gap ($-V_p$ to 0), the solution obtained represents an interface state. Because $V_p$ is only of the order 40 meV, the interface state has very long decay lengths, $\lambda$, in both HgTe $[\lambda_A = \hbar/(2m_A|E_0|)^{1/2}]$ and CdTe $[\lambda_B = \hbar/(2|m_B(E_0+V_p)|)^{1/2}]$.

The above analysis ignores the presence of heavy-hole bands. In HgTe the heavy-hole valence band is degenerate with the conduction band at $\Gamma$. The heavy-hole band overlaps the gap between $-V_p$ and 0 and the interface state can couple to a HgTe propagating heavy-hole state. It is thus not completely localized at the interface and should more accurately be denoted a quasi-interface state or interface resonance. It is not clear how such coupling affects the interface state unless a more realistic model is considered. We, therefore, performed a nearest-neighbor tight-binding calculation using the recently developed "reduced Hamiltonian method."[7] The method allows us to study superlattices of arbitrary layer thickness with a modest computational effort in a ten-band model. The tight-binding parameters were chosen to produce realistic band gaps, spin-orbit splittings, and effective masses for the conduction, light-hole, and heavy-hole bands. The results are compared with those obtained by Bastard's envelope-function method.[5] Both calculations predict the existence of quasi-interface states and the energies produced by the two methods agree well.

Figure 1(a) shows the dispersion curves of the quasi-interface states in HgTe-CdTe (001) superlattices with $M = 10$ and $N = 30$, 40, 50, and 100 (where $M$ and $N$ are numbers of atomic layers of CdTe and HgTe, respectively, in the direction perpendicular to the superlattice interfaces). The solid and dashed curves are obtained by the envelope function method and the dotted curves (for positive energy states only) by the tight-binding method. Note that in the envelope-function method,[5] and band gaps and effective masses are related by $\epsilon_B/\epsilon_A = m_B/m_A$, where $A$ and $B$ denote HgTe and CdTe, respectively. Given that $\epsilon_A = -0.3$ eV, $m_A = 0.026m_0$, and $m_B = -0.103m_0$,[8] we are forced to choose $\epsilon_B \simeq 1.2$ eV (instead of the experimental value 1.6 eV). The discrepancy should not affect the results for superlattice states with energies near the top of the valence band.

 

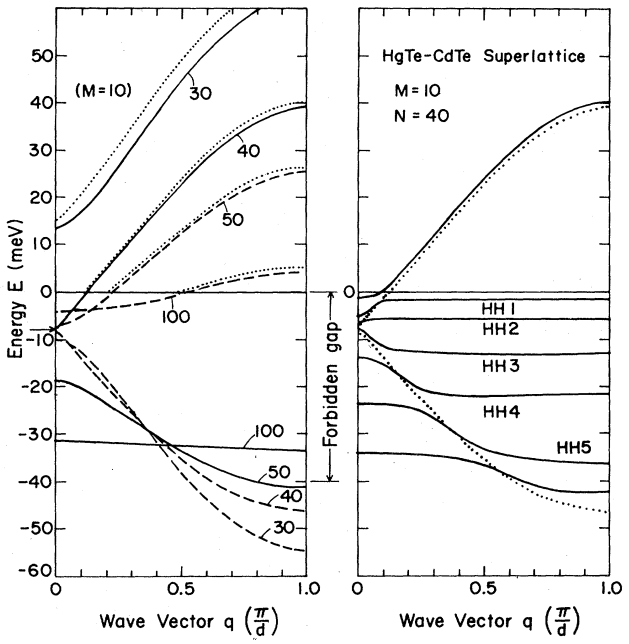


FIG. 1. (a) Dispersion curves of interface states in HgTe-CdTe superlattices with $M=10$ and $N=30$, 40, 50, and 100, calculated by the tight-binding method (for positive-energy states) (dotted) and the envelope-function method (dashed and solid). (b) Dispersion curves of interface and heavy-hole subbands in the (40/10) HgTe-CdTe superlattices calculated by the tight-binding method. The dotted curves denote results of the envelope-function method. The symbol HHn denotes the $n$th heavy-hole subband. $d$ is the length of the superlattice unit cell.

The energy region where no propagating bulk conduction or light-hole states are allowed is marked "forbidden gap." The arrow points to the energy position ($\simeq -8$ meV) of the interface state predicted by (1). In the superlattice, the interaction between the quasi-interface states at the two interfaces in each superlattice unit cell leads to two interface bands. The interface band whose $p$-component envelope function at $q=0$ is symmetric (antisymmetric) is shown in Fig. 1(a) as a dashed (solid) line. Note that at $q\neq 0$ they are neither symmetric nor antisymmetric. For $N \gtrsim 40$, both interface bands fall within the forbidden gap near $q=0$. One goes above zero and becomes a propagating state for $q>0$. The other either goes below $-V_p$ for $q>0$ or remains within the gap for all $q$. For $N=30$, the higher interface band lies above zero for all $q$. The dispersion curves for interface states with positive energies obtained in the two methods agree quite well. For interface states with negative energies, the tight-binding calculation predicts strong hybridization with heavy-hole subbands resulting in gaps where the interface band would intersect the heavy-hole bands in the envelope function model. Hence, the dispersion curves are more complicated. An example (for $N=40$) is shown in Fig. 1(b). Here, we find that the mixing between the interface state and the heavy-hole subband states modifies the valence-band dispersion curves considerably.

If we consider a model semiconductor in which the heavy-hole band is absent, then by symmetry argument it can be shown that one interface band will be occupied and the other empty. Thus, in the HgTe-CdTe superlattice, the higher interface band represents a conduction subband whereas the lower interface band represents a valence subband.

The optical and transport properties of the HgTe-CdTe superlattice depend strongly on whether or not the energy of the higher interface band is either higher than or within the forbidden gap shown in Fig. 1. If it is higher than the gap for all $q$, the superlattice is a semiconductor with the semiconducting gap occurring between the higher interface band and the first heavy-hole subband. If any part of the higher band lies at least slightly within the gap, the superlattice is a metal. This is because the energy of the uppermost heavy-hole superlattice state is within a few millivolts below the top of the gap. The portion of the higher interface band with energy below the heavy-hole band will be filled and the portion above will be empty of carriers, forming a partially filled band and thus a metal. However, if one takes into account the hybridization between the interface band and heavy-hole subbands as shown in Fig. 1(b), then the superlattice behaves like a semiconductor with a band gap on the order of a few meV, depending on the strength of the hybridization.

Since the optical properties depend strongly on the superlattice wave functions, it is important to understand them. First we consider the wave functions of the quasi-interface states obtained in the envelope-function model.[5] In this model each superlattice state has two components: the $s$ like and the $p$ like. For superlattice states with energies close to zero the envelope function is predominantly $p$ like, since both the HgTe conduction-band and the CdTe valence-band states are mainly $p$ like at small $\mathbf{k}$. We find that for $N/M \gtrsim |m_B/m_A| = 4$, the interface state at $q=0$ with symmetric $p$ component lies higher in energy than the other interface state, while for $N/M \lesssim |m_B/m_A|$, the situation is reversed. Hence, a crossing of the energy levels of the two interface states occurs as we vary the value of $N$, while keeping $M$ fixed. This is demonstrated in Fig. 2 in which the energies of the two interface states at $q=0$ are plotted as functions of the number of HgTe atomic layers ($N$) for fixed number of CdTe atomic layers ($M=5$, 10, and 20).

The fact that the ordering of the two interface states is inverted at some $N$ for each fixed $M$ can be qualitatively understood as follows. The energy of a superlattice state is determined by the sum of kinetic energies in HgTe and CdTe. In the one-band model, the wave functions of the two interface states are symmetric and antisymmetric combinations of two $p$-like envelope functions localized at the two interfaces. If we let $M \gg N$, then the kinetic energies in CdTe for symmetric and antisymmetric combinations are approximately the same (because the cross term becomes vanishingly small); hence, the kinetic energy in HgTe plays the determining role. The cross term which determines the energy splitting of the two interface states is given by

$$\frac{1}{2m_A}\int_0^{l_A} \exp[-b(l_A-z)]p_z^2\exp(-bz)\,dz \quad (b\equiv|k_A|)$$

and is negative. Thus, the state with symmetric $p$ component lies lower in energy. In the opposite limit $N \gg M$, the kinetic energy in CdTe plays the determining role. The cross term which determines the splitting is given by a similar integral but with the index $A$ replaced by $B$. But since $m_B$ is now negative, the cross term becomes positive and

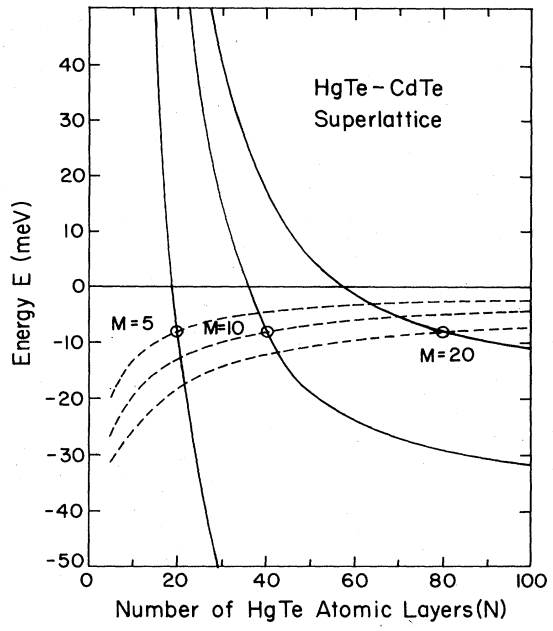


FIG. 2. Energies of interface states with symmetric (dashed) and antisymmetric (solid) $p$-component envelope functions calculated in Bastard's model are plotted as functions of the number of HgTe atomic layers ($N$) for fixed number of CdTe atomic layers ($M=5$, 10, and 20). The circles indicate the positions where two interface states of opposite symmetries cross.

the state with symmetric $p$ component lies higher in energy. It is instructive to note that the $M >> N$ case describes a CdTe-HgTe-CdTe double heterostructure whereas the $N >> M$ case describes a HgTe-CdTe-HgTe double heterostructure. In the one-band model, the second double heterostructure is analogous to the first except that its energy band diagram is inverted and the effective masses are different. The symmetric and antisymmetric interface states are in fact the ground and first excited states that are bound to the HgTe quantum well in the first double heterostructure. In the second double heterostructure, the ordering of all energy levels is inverted.

The analysis of the superlattice wave function in the tight-binding model is somewhat more complicated due to the mixing with heavy-hole subbands. Each superlattice state now has five components related to the atomic orbitals used in the tight-binding model. However, for the states of interest here, there are only three dominating components: $s$ like, light hole like (LH), and heavy hole like (HH) defined as the orbital combinations: $s\uparrow$, $[2z\downarrow+(x-iy)\uparrow]/\sqrt{6}$, and $-(x+iy)\uparrow/\sqrt{2}$, respectively. For the case that the interface state has no appreciable mixing with the heavy-hole state, the wave function is very similar to that obtained in Bastard's model. When substantial mixing between the interface state and heavy-hole state occurs, the wave function contains a HH component of opposite parity to that of the LH component. The reason that LH and HH components of opposite parities mix was previously discussed.[9]

When the superlattice is a semiconductor, i.e., the higher interface band lies above 0 eV for all $q(N/M<4)$, we find that the higher interface state at $q=0$ always contains an antisymmetric $p$ component and some appreciable fraction of a symmetric $s$ component. Since the lower interface state contains mainly symmetric $p$ component, the optical matrix element between the two states is appreciable. Furthermore, since the highest heavy-hole state is $p$ like and symmetric, we also expect appreciable optical transition from the heavy-hole subband to the conduction subband.

We have calculated the optical matrix elements for interband transitions in the HgTe-CdTe superlattice. In Table I we list the squared matrix elements

$$Q_{\parallel}\equiv\frac{2}{m_0}(|\hat{\mathbf{x}}\cdot\mathbf{P}_{vc}|^2+|\hat{\mathbf{y}}\cdot\mathbf{P}_{vc}|^2)$$

and

$$Q_{\perp}\equiv\frac{2}{m_0}|\hat{\mathbf{z}}\cdot\mathbf{P}_{vc}|^2$$

for optical transitions from the lower interface state [denoted $Q_{\parallel}(\mathrm{I})$ and $Q_{\perp}(\mathrm{I})$] and the highest heavy-hole state [denoted $Q_{\parallel}(\mathrm{HH})$] to the lowest conduction (higher interface) state for a number of HgTe-CdTe superlattices. Here, $\mathbf{P}_{vc}$ is the momentum matrix element and $\hat{\mathbf{x}},\hat{\mathbf{y}},\hat{\mathbf{z}}$ denote the directions of polarization of light ($\hat{\mathbf{z}}$ is perpendicular to the interface). Note that $Q_{\perp}$ for the heavy-hole state is vanishingly small and is not listed. The superlattice energies $E_c$, $E_{\mathrm{HH}}$, and $E_{\mathrm{I}}$ for the conduction, heavy-hole, and lower interface states, respectively, are also listed for reference. The corresponding result for a $Hg_{0.77}Cd_{0.23}Te$ alloy is also included for comparison. As seen in Table I, the total squared optical matrix element $(Q_{\parallel}+Q_{\perp})$ for the interface–conduction-band transition is comparable to that for the heavy-hole–conduction-band transition, while the polarization dependences are quite different. Thus, the interface

TABLE I. Squared optical matrix elements [in units of $E_P\equiv(2/m_0)|\langle s|P_x|x\rangle|^2$ for HgTe] for transitions from the lower interface state and the highest-energy heavy-hole state to the lowest-energy conduction state (higher interface state), in a number of HgTe-CdTe superlattices. The last row shows the corresponding result for a $Hg_{1-x}Cd_xTe$ alloy with $x=0.23$.

| $(N/M)$ | $E_c$ (meV) | $E_{\mathrm{HH}}$ (meV) | $E_{\mathrm{I}}$ (meV) | $Q_{\parallel}$ (HH) | $Q_{\parallel}$ (I) | $Q_{\parallel}$ (I) |
|---|---|---|---|---|---|---|
| 4/9 | 110.0 | −8.7 | −10.0 | 0.76 | 0.24 | 0.47 |
| 6/13 | 93.0 | −7.0 | −10.3 | 0.61 | 0.19 | 0.37 |
| 8/15 | 97.9 | −6.3 | −11.3 | 0.52 | 0.16 | 0.30 |
| 10/17 | 93.0 | −5.5 | −11.9 | 0.45 | 0.13 | 0.24 |
| 15/19 | 94.4 | −4.8 | −13.4 | 0.37 | 0.08 | 0.15 |
| 18/20 | 91.0 | −4.5 | −13.7 | 0.34 | 0.06 | 0.11 |
| alloy | 107.4 | 0 | . . . | 1.03 | . . . | . . . |

state described here plays an important role in determining the optical properties of HgTe-CdTe superlattices. We find that the squared optical matrix element increases with decreasing ratio of $N/M$ due to the increasingly large percentage of the symmetric $s$-like component in the conduction state envelope function.

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[1]J. N. Schulman and T. C. McGill, Appl. Phys. Lett. **34**, 663 (1979).
[2]J. P. Faurie, A. Millon, and J. Piaguet, Appl. Phys. Lett. **41**, 713 (1982).
[3]Y. Guldner, G. Bastard, J. P. Vieren, M. Voos, J. P. Faurie, and A. Millon, Phys. Rev. Lett. **51**, 907 (1983).
[4]P. P. Chow and D. Thomson, in Proceedings of the 1984 U.S. Workshop on Physics and Chemistry of Mercury Cadmium Telluride, 1984 (unpublished).
[5]G. Bastard, Phys. Rev. B **25**, 7584 (1982); D. L. Smith, T. C. McGill, and J. N. Schulman, Appl. Phys. Lett. **43**, 180 (1983).
[6]G. Wu, C. Mailhiot, and T. C. McGill, in Proceedings of the First International Conference on Superlattices, Microstructures, and Microdevices, Urbana-Champaign, 1984 (unpublished).
[7]J. N. Schulman and Y. C. Chang, Phys. Rev. B **24**, 4445 (1981).
[8]P. Lawaetz, Phys. Rev. B **4**, 3460 (1971).
[9]Y. C. Chang and J. N. Schulman, Appl. Phys. Lett. **43**, 536 (1983); and (unpublished).