Subband structure of strained-layer CdTe/ZnTe superlattices: A reexamination

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With recent new values of the CdTe deformation potentials, we present a reexamination of the combined effects of band offsets and lattice mismatch on the subband structure of strained-layer CdTe/ZnTe superlattices. It is shown that the subband structure of these superlattices is very sensitive to the strain parameters. The value $\Delta E_v = 55 \pm 40$ meV is obtained for the zero-strain valence-band offset and a relation between the CdTe (N_1) and ZnTe (N_2) monolayer numbers of the strained-layer superlattice $(\mathrm{CdTe})_{N_1}/(\mathrm{ZnTe})_{N_2}$ giving rise to a degenerate band gap $[E(C1H1)=E(C1L1)]$ is proposed, $N_1 \times N_2 \simeq 30$. For $N_1 \times N_2 < 30$, the band gap is $E(C1H1)$, and the superlattice has a type-I configuration; for $N_1 \times N_2 > 30$, the band gap is $E(C1L1)$, and the superlattice has a type-II configuration.

In recent years, tremendous developments have occurred in the field of strained-layer superlattices (SLS's) due to both their intrinsic interest and possible applications as electronic devices. In these SLS's, the lattice mismatch is accommodated by a uniform lattice strain and the resulting so-called "pseudomorphic interface" is characterized by an in-plane lattice constant. In this case, the hole subband structure results from the combined effects of the zero-strain valence-band offset and lattice mismatch. The electron and hole potential wells may be written as

$$V_e = K\,\Delta E_g + \Delta V_e \ , \tag{1a}$$

$$V_{\mathrm{hh}} = (K-1)\Delta E_g + \Delta V_{\mathrm{hh}} \ , \tag{1b}$$

$$V_{\mathrm{lh}} = (K-1)\Delta E_g + \Delta V_{\mathrm{lh}} \ , \tag{1c}$$

where ΔE_g is the band-gap offset. K characterizes the zero-strain band offsets, $\Delta E_c = E_{c2} - E_{c1} = K\,\Delta E_g$ and $\Delta E_v = E_{v2} - E_{v1} = (K-1)\Delta E_g$. ΔV_i ($i = e$,hh,lh) are the strain contributions to the electron and hole potential wells, where hh and lh denote heavy hole and light hole respectively.

Concerning the CdTe/ZnTe superlattices, it is worth noting that, on account of the common anion rule, the zero-strain valence-band offset is expected to be small; on the other hand, on account of the very important lattice mismatch, $\Delta a/a \simeq 6.2\%$, the strain-induced splitting of the valence bands may be relatively important. Moreover, if the first effect is an intrinsic one, the lattice-mismatch effect is a function of the layer thicknesses. So, depending on the layer thicknesses, the difference between the zero-strain valence-band offset and the strain-induced splitting of the valence-band may induce a reversal of energy position of the heavy- and light-hole subbands.

In a previous paper[1], we have presented a detailed investigation of such effects and have shown that, depending on the relative values of these two effects, the SLS's may either be type I for the electron–heavy-hole system and type II for the electron–light-hole system; or type I or II for both systems. Moreover, the deformation potentials of both CdTe and ZnTe must be accurately known. A reliable value of the hydrostatic deformation potential of the band gap for ZnTe exists. It was measured recently by Strossmer *et al.*,[2] at room temperature in a diamond anvil cell for pressures up to the second phase transition (~20 GPa). The shear deformation potential b, on the other hand, has been measured by Wardzynski *et al.*[3] for CdTe the situation is not so clear. The only data concerning the shear deformation potentials of the valence band, have been obtained by Thomas[4] from uniaxial stress measurements. Now, probably because the elastic compliance constants of CdTe are very important and/or because the quality of the material was not very good, it was very difficult to perform reliable uniaxial stress measurements. This clearly appears on the dispersion of the experimental results given by Thomas (see Table I of Ref. 4). In our preceding work, we have used the hydrostatic deformation potential of the band gap of CdTe measured by Babonas *et al.*,[5] and renormalized the experimental data of Thomas in order to obtain the deformation potentials given in Table I of Ref. 1.

In this Brief Report, we reexamine our experimental data concerning the CdTe/ZnTe SLS's with new values of the CdTe deformation potentials. Dunstan *et al.*[6] have measured the hydrostatic deformation potential of the direct band gap of CdTe by observing the pressure dependence of the free-exciton luminescence and of the donor-acceptor pair luminescence under hydrostatic preassure up to 35 kbars at 2 K. The value $dE/dP = 6.5 \pm 0.2$ meV/kbars was obtained corresponding to a hydrostatic-

deformation-potential value $a=-2.74\pm0.09$ eV. Concerning the shear deformation potential of the Γ_8 valence band, we have developed and carried out a new technique which consists of measuring the ratio of the piezomodulation of light- and heavy-hole states under a coplanar periodic stress. In a previous paper[7] we reported a differential-spectroscopy investigation of good-quality GaAs/$Ga_{1-x}Al_{1-x}As$ quantum wells and we have shown that the piezomodulation technique is a powerful tool in order to identify heavy- and light-hole states in quantum wells and superlattices. Conversely, measuring the ratio of the piezoreflectivity spectra associated to splitted heavy- and light-hole states permits an accurate determination of the shear deformation potential of the Γ_8 valence band. The ratio of the piezomodulation parameters of the light- and heavy-holes transitions are given by[7]

$$R=\frac{dE_{e\text{-lh}}/dX}{dE_{e\text{-hh}}/dX}=\frac{2a(S_{11}+2S_{12})+b(S_{11}-S_{12})}{2a(S_{11}+2S_{12})-b(S_{11}-S_{12})}\ . \quad (2)$$

In CdTe the shear deformation potential b is very important, so that the denominator of Eq. (2) is close to zero, and the value of the ratio is very sensitive to the value of b. As a result, and specially for CdTe, this technique permits an accurate determination of b. This has been studied elsewhere;[8] the ratio $R=-16$ was measured and the value $b=-1.0\pm0.1$ eV was deduced. Lastly, concerning the respective valence (a_v) and conduction (a_c) contributions to the band-gap hydrostatic deformation potential (a) we used, for both ZnTe and CdTe, the ratio proposed by Camphausen *et al.*[9] recently confirmed from tight-binding calculation by Dunstan *et al.*[6]. All values of the parameters used in this Brief Report are summarized in Table I, where the deformation potentials used in Ref. (1) for CdTe, and those proposed by Thomas (Ref. 4) have been reported for clarity.

Now, using these new values of the deformation potentials of CdTe, conduct to revise the interpretation of our experimental data is given in Ref. 1. For all samples we compare the experimental value of the transition energies with the $E(C1H1)$ and $E(C1L1)$ energy gaps calculated in the framework of the Kronig-Penney model with the mass parameters given in Table I. Typical curves are given in Fig. 1. The experimental values appear as solid

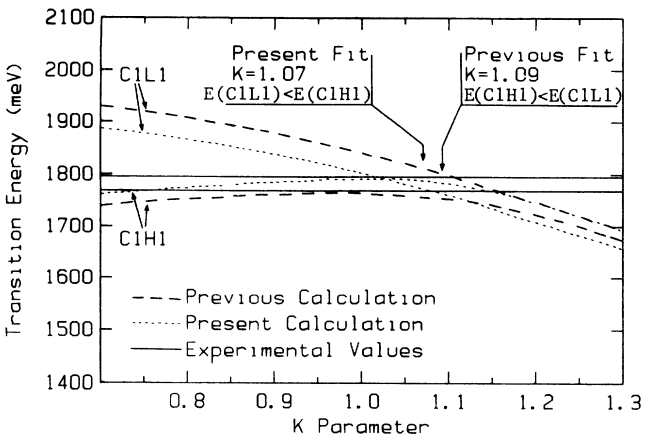

FIG. 1. Comparison of the measured (solid lines) and calculated (dashed lines, previous strain parameters; dotted lines, present strain parameters) values of the $E(C1H1)$ and $E(C1L1)$ transition energies on sample 3.

horizontal lines, and the calculated values as a function of the valence-band offset (K parameter) appear as dashed-lines (previous strain parameters) and dotted-lines (present strain parameters). Clearly the best fit is now obtained with $K=1.07$. This shows that the ground state of the valence band is the light-hole band, instead of the heavy-hole one. The band gap is $E(C1L1)$ and the superlattice has a type-II configuration, with the electrons mostly localized in the CdTe layers and the light holes preferentially localized in the ZnTe layers. The high-energy structure which is now the $C1H1$ transition corresponds to a type I transition with both the electron and the heavy hole preferentially localized in the CdTe layers.

Figure 1 clearly shows that the behavior of the structures, especially the crossover of the light- and heavy-holes states, is very sensitive to the strain parameters. All the experimental data concerning the samples are investigated in Ref. 1, and the corresponding transition energies calculated with the new strain parameters are summarized in Table II. for the valence-band offset, we deduce a mean value $\Delta E_v=55\pm40$ meV, which is close to the one proposed in Ref. 1.

Now, by using these new values for the strain parame-

TABLE I. Parameters used in the calculations.

Parameters	Present calculation	CdTe Ref. 1	CdTe Ref. 4	ZnTe Present calculation
me/m_0	0.099 (Ref. 10)			0.116 (Ref. 10)
γ_1	4.11 (Ref. 10)			4.07 (Ref. 10)
γ_2	1.08 (Ref. 10)			0.78 (Ref. 10)
γ_3	1.95 (Ref. 10)			1.59 (Ref. 10)
S_{11} (10^{-6} bars^{-1})	3.58 (Ref. 11)			2.38 (Ref. 3)
S_{12} (10^{-6} bars^{-1})	−1.39 (Ref. 11)			−0.86 (Ref. 3)
a (eV)	−2.74 (Ref. 6)	−3.33	−2.6	−5.3 (Ref. 2)
a_c (eV)	−1.80	−2.15		−3.5
a_v (eV)	0.94	1.18		1.80
b (eV)	−1.0 (Ref. 8)	−1.4	−2.7	−1.3 (Ref. 3)

TABLE II. Experimental and calculated values of the $E(C1H1)$ and $E(C1L1)$ energy gaps (in eV). The K value and the associated ΔE_v valence-band offset (in meV) correspond to the better fit. The sample characteristics are given in Ref. 1.

Sample	(N_1,N_2)	Experiment (eV)	Calculated values $E(C1H1)$ (eV)	Calculated values $E(C1L1)$ (eV)	K	ΔE_v (meV)
No. 1	(6,6)	1.840	1.84		1.05	43
		1.800		1.84		
No. 2	(9,12)	1.780	1.77		1.07	55
		1.747		1.74		
No. 3	(8,7)	1.795	1.79		1.07	55
		1.768		1.77		
No. 4	(8,10)	1.840	1.80		1.09	71
		1.795		1.80		
No. 5	(6,10)	1.855	1.86		1.12	94
		1.820		1.83		
No. 6	(8,11)	1.820	1.80		1.06	47
		1.784		1.78		
No. 7	(10,12)	1.765	1.75		1.04	34
		1.736		1.73		

ters and valence-band offset, we could calculate for the (N_1,N_2) pair [N_1=CdTe monolayer number and N_2=ZnTe monolayer number in the SLS $(CdTe)_{N_1}/(ZnTe)_{N_2}$] the series of values giving rise to a degenerate band gap for the superlattice: $E_g=E(C1H1)=E(C1L1)$. The result is illustrated as a dottted-dashed line in Fig. 2. Below this line the ground state of the valence band is the heavy-hole subband, the band gap is $E_g=E(C1H1)<E(C1L1)$, and the superlattice has a type-I configuration. Above this line, the ground state of the valence band is the light-hole subband, the band gap is $E_g=E(C1L1)<E(C1H1)$, and the superlattice has a type-II configuration. The isoenergy gaps are illustrated by solid lines which correspond to $E(C1H1)$ [$E(C1L1)$] transitions below (above) the dotted-dashed line. When they are not fundamental gaps, they have been indicated as dotted lines.

Figure 2 is to be compared with Fig. 7 of Ref. 1. Clearly, it confirms that the behavior of the superlattice, as a function of the CdTe and ZnTe monolayer numbers, is very sensitive to the strain parameters. This results from the three following reasons. (i) The lattice mismatch between CdTe and ZnTe is very important ($\Delta a/a=6.2\%$) and gives rise to a very important interface coplanar stress, about 15 kbars, (ii) the valence-band

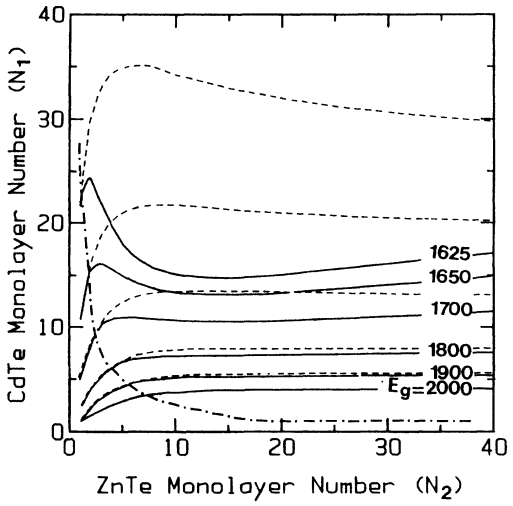

FIG. 2. Low-temperature $(CdTe)_{N_1}/(ZnTe)_{N_2}$ superlattice band gap as a function of CdTe (N_1) and ZnTe (N_2) monolayer numbers per superlattice period. The dotted-dashed line corresponds to the $E(C1H1)-E(C1L1)$ crossing. Below (above) this line the band gap corresponds to the $E(C1H1)$ [$E(C1L1)$] transition and the superlattice has a type-I (-II) configuration. Solids lines correspond to isoenergy gaps.

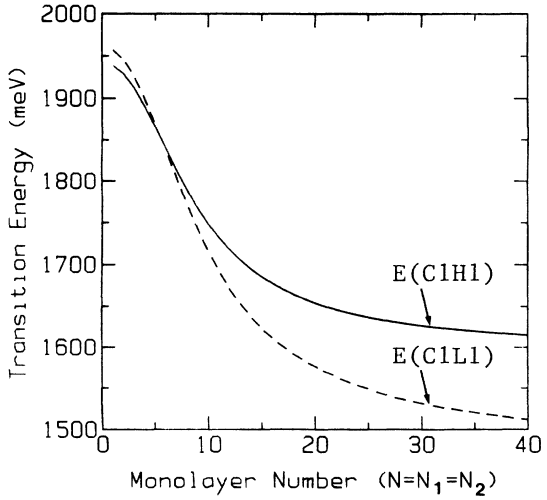

FIG. 3. N dependences of the $E(C1H1)$ and $E(C1L1)$ transition energies for symmetric $(N=N_1=N_2)$ $(CdTe)_N/(ZnTe)_N$ superlattices.

stress-splitting of CdTe is very important, about 10 meV/kbars, and (iii) the zero-strain valence-band offset between CdTe and ZnTe is very small (about 55 meV). As a result, the strain splitting is more important than the zero-strain valence-band offset, and the hole levels pattern is completely reorganized by the strain field.

It appears from Fig. 2 that, if we consider symmetric superlattices with equal monolayer numbers $N=N_1=N_2$, short-period superlattices ($N<5$) have a type-I configuration with the heavy hole as the hole ground state; on the contrary, large-period superlattices ($N>6$) have a type-II configuration with the light hole as the hole ground state. The curve giving rise to a degenerate band gap [$E(C1H1)=E(C1L1)$] may be approximated by the relation $N_1 \times N_2 \simeq 30$. This is illustrated in a somewhat different way in Fig. 3, where we show the N dependence of the $E(C1H1)$ and $E(C1L1)$ transition energies for symmetric superlattices.

In conclusion, and beyond the scope of the CdTe/ZnTe superlattices, it is worth noting that before any study of strained-layer structures with small valence-band offset (like II-VI heterostructers with a common anion), a careful investigation of the deformation potentials for each compound should be done.

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