

Exciton binding energies and the valence-band offset in mixed type-I–type-II strained-layer superlattices

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Strained CdTe-Cd_{1-x}Zn_xTe superlattices are of mixed type: electrons and heavy holes are confined to the CdTe layers (type I) while light holes are confined to the Cd_{1-x}Zn_xTe layers (type II). In this paper we calculate the exciton binding energy (EBE) as a function of superlattice period for both type-I (spatially direct) and type-II (spatially indirect) excitons. For the heavy-hole (type-I) exciton the binding energy is larger than the bulk value, and varies only slowly with the period down to small periods, where the exciton acquires a three-dimensional character and our calculation breaks down. For the light-hole (type-II) exciton the binding energy at large period is much smaller, due to the spatial separation of electron and hole. As the period decreases, the binding energy increases steadily to reach its bulk value for vanishingly small period. Given the EBE's, we can fit the already published data on the exciton transition energies with a single adjustable parameter, the "average valence-band offset" (averaged over the heavy and light holes). This is the algebraic sum of the chemical-offset and the hydrostatic-strain contribution, and is found to be (2±4)% of the difference in band gap between the barrier and well. This value lies in the range predicted theoretically.

INTRODUCTION

Excitons in semiconductor quantum wells (QW's) and superlattices (SL's) have received considerable attention in the last few years.¹⁻⁸ Most studies have been done in type-I structures where the electrons and the holes are confined to the same material, so that the exciton is spatially direct. In this case it has been shown that the exciton binding energy (EBE) may increase by a large factor relative to its bulk value when the carriers are confined in quantum wells with thicknesses of the order of the Bohr radius. In quantum wells of smaller thickness or in small period SL's the carriers are less confined and the binding energy decreases toward its bulk value. The situation is quite different in type-II SL's where the electrons and holes are spatially separated, being confined in different materials, and the exciton is spatially indirect. Then the Coulomb interaction is reduced and, as shown by several theoretical studies, the binding energy may be considerably reduced below its value in the equivalent bulk alloy. Its variation with the SL period is opposite to the case of the type-I structures. For short period SL's the binding energy increases toward its value in the bulk.

Most studies of the EBE in type-II structures^{1,2,5,7} have been carried out on the GaAs/AlAs system. In this case the situation is somewhat complicated since the exciton in these structures is indirect in momentum space as well as in real space, and the validity of the effective-mass

approximation is questionable. Moreover the SL is type II only in a limited range of quantum well and barrier thicknesses. In this paper we describe a study of the EBE's of CdTe/Cd_{1-x}Zn_xTe ($x \approx 0.08$) SL's and multiple quantum wells (MQW) where type-II excitons can be observed over a wide range of SL periods extending from the MQW regime, with QW thicknesses larger than the exciton Bohr radius, to short period SL's whose behavior approaches that of the equivalent bulk alloy. In a previous paper⁴ we have shown that these strained structures are of mixed type: both the electron and the heavy holes are confined to the CdTe layers (type I), but the light holes are in the Cd_{1-x}Zn_xTe layers, resulting in a type-II SL. This is due to the fact that, as we shall see, most of the valence-band offset (VBO) results from strain.⁹ The absolute value of the "chemical" VBO (i.e., the VBO in the absence of strain) at the CdTe/Cd_{1-x}Zn_xTe interface is extremely small, less than 10% of the band-gap difference ΔE_g . The CdTe and Cd_{1-x}Zn_xTe being in biaxial compression and dilatation, respectively, the heavy-hole–light-hole splitting has the opposite sign in the two materials, and since the chemical VBO is small the heavy and light holes are confined to the CdTe and Cd_{1-x}Zn_xTe layers, respectively.

Evidence for a small VBO has been obtained from optical studies of heterostructures with x values ranging from 0.08 to 1.^{4,10-12} The most reliable data are those for small x (0.08–0.13) since the optical transitions are then

sharp and the heavy- and light-hole excitonic transitions can be clearly identified by polarized photoluminescence excitation spectroscopy and by piezorefectivity. On the other hand, a recent paper¹³ obtains a chemical VBO of about 20% of ΔE_g from an analysis of oscillator strengths, estimated from photoluminescence excitation spectra, of light- and heavy-hole excitons in a separate confinement quantum well heterostructure. This result is at variance with a large body of data, including those of the present paper. Possible reasons for this discrepancy will be discussed elsewhere.

While there is little doubt that the VBO is small, the precision with which it can be determined from optical data is limited by the accuracy with which the EBE's for the light- and heavy-hole excitons are known, since they are comparable in magnitude to the VBO. In this paper we make a careful calculation of these binding energies, and thus can make a more precise estimate of the VBO than was previously possible. We compare our result with recent calculations,^{14,15} in some of which the effect of hydrostatic deformation is taken into account more accurately than has previously been the case.

In Ref. 4 we described a detailed optical study of a series of SL's with periods ranging from 60 to 400 Å. In the present paper we will first recall the main characteristics of these structures and the results of the optical studies. Since the optical data give the energies of free excitons, they have to be corrected for the EBE's in order to obtain the lowest subband positions. In this paper we present the model used for the calculations of these binding energies, and show that they are relatively insensitive to the parameters assumed, in particular to the valence-band offset. The energy positions of the heavy- and light-hole subband edges, relative to the lowest conduction subband, can thus be obtained from the observed spectra with a precision of 1 to 2 meV. We then fit these positions to a calculation of the subband energies in which the average VBO is the only free parameter.

The VBO's for the heavy and light holes have three components. The first is due to the shear strain, which is approximately equal and opposite in the well and in the barrier in all the samples considered here. Since the shear deformation potential is known, this component is known. The second component is the so-called chemical offset ΔV_v , which is the negative of the difference between the ionization potentials of the isolated unstrained materials (with this definition ΔV_v is positive for a type-I structure). It is this component of the offset which is obtained, for instance by Tersoff¹⁴ and by van de Walle,¹⁵ in "first-principles" calculations. It is often expressed as a fraction α of the energy gap difference ΔE_g between the well and barrier. While this can be misleading, since α is not in general independent of the composition, it is adequate for the small values of x (the fractional Zn content of the barrier) considered here. The third component is a hydrostatic strain term which depends on the *absolute* deformation potential a_v of the valence bands of the two materials. These absolute deformation potentials are not accessible by piezospectroscopic experiments, which measure the *relative* deformation potential, $a = a_c - a_v$, of the conduction- and valence-band edges in the same material.

However, several "first-principles" calculations of a_v exist, of which the most recent is that of van de Walle.¹⁵ The second and third components cannot be separated by measurements of the type discussed here, since there is no absolute energy reference point, such as the vacuum level, and there is no reason to trust the calculations of a_v more or less than those of ΔV_v (Ref. 16) (this fact, which is carefully discussed by van de Walle, has not always been clearly recognized in the experimental literature). We will call the sum of these two components the "average band offset" ΔV_a , the "average" being over the light- and heavy-hole band edges. Note that the conduction-band offset is determined by ΔV_a , since ΔE_g and a are known. Since, for small x , ΔV_a is proportional to x , we are left with one fitting parameter, the ratio $\Delta V_a/x$.

EXPERIMENT

The samples were grown in a Riber 32P machine on $\langle 001 \rangle$ oriented $\text{Cd}_{1-y}\text{Zn}_y\text{Te}$ substrates. Reflection high-energy electron diffraction¹⁷ (RHEED) was used to optimize the two-dimensional layer by layer growth of CdTe and the $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ alloy and to measure the layer thickness to one monolayer accuracy; the SL period, the alloy composition, and the strain in the QW and barrier layers were precisely determined from x-ray data. Most of the samples discussed in this paper consist of equal thickness layers of CdTe and $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ ($x \approx 0.08$) grown on a $\text{Cd}_{1-y}\text{Zn}_y\text{Te}$ ($y \approx 0.04$) substrate. Then the strains in the CdTe and $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ layers are equal and opposite, so that strain is symmetrized in the way well known in the InAs/GaAs (Ref. 18) and Si/Ge (Ref. 19) systems, and thick SL's can be coherently grown. For SL's with unequal QW and barrier thicknesses or larger zinc content in the barrier, the number of periods was chosen small enough to avoid relaxation of the structures. The structural parameters of these samples are summarized in Table I. The optical study of these samples includes transmission, reflectivity, luminescence, and photoluminescence excitation (PLE) spectra. The high quality of the structures is shown by the small linewidth and the very small Stokes shift. Transitions related to the light-hole exciton were distinguished from heavy-hole ones by polarized photoluminescence excitation.^{4,20} For these structures with a small zinc content ($x \approx 0.08$) in the barrier, the offset is small, and for QW's with a period smaller than 170 Å only one bound electron state exists. The energies of the e_1h_1 and e_1l_1 exciton lines are given in Table I.

ANALYSIS

The observed 1s exciton energy for the spatially direct (heavy-hole) and indirect (light-hole) transitions may be expressed as

$$E(e_1h_1) = E_g + \Delta V_g - \Delta V_h + E_c(E_1) + E_c(H_1) - E_{Xh} \quad (1)$$

$$E(e_1l_1) = E_g + \Delta V_g - \Delta V_a - \Delta V_l + E_c(E_1) + E_c(L_1) - E_{Xl} \quad (2)$$

TABLE I. Sample parameters. L_w and L_b are the quantum well and barrier widths. $E(e_1h_1)$ and $E(e_1l_1)$ are the exciton energies observed in PLE spectra (from Refs. 4 and 20).

Sample number	% Zn substrate	% Zn barrier	L_w (Å)	L_b (Å)	Period (Å)	$E(e_1h_1)$ (meV)	$E(e_1l_1)$ (meV)
3	4.50	8.60	140	138	278	1601.70	1611.50
5	4.40	9.90	128	126	254	1603.30	1610.60
6	4.55	8.25	71	138	209	1613.00	1618.20
1	4.50	10.30	71	73	144	1612.00	1616.60
4	4.50	9.30	61	60	121	1615.00	1618.10
2	3.45	8.70	32	35	67	1618.75	1616.00

Here $E_g = 1.606$ eV is the band gap of bulk CdTe, ΔV_g the hydrostatic strain shift of the conduction-band edge in the CdTe layer relative to the valence band, ΔV_a the average VBO defined above, ΔV_h the shear strain shift of the heavy-hole band in the CdTe layer, and ΔV_l that of the light-hole band in the $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ layer. Note that our definitions of the quantities ΔV_h and ΔV_l differ slightly from those used previously (e.g., in Ref. 4), in that only the shear strain contribution is included. $E_c(E_1)$, $E_c(H_1)$, and $E_c(L_1)$ are, respectively, the electron, heavy-hole, and light-hole confinement energies in the $n=1$ subband, and E_{xh} and E_{xl} are the respective EBE's.

Most of the parameters (QW and barrier widths, zinc concentration in the barriers and in the substrate) involved in this calculation are very well known (as shown, for example, by the excellent agreement between their RHEED and x-ray determination¹⁷). For these coherently grown structures the strains in the barrier and QW layers are also accurately known, as are the spectroscopically accessible deformation potentials and the effective masses. Thus the only unknown parameter is ΔV_a , the offset at the CdTe/ $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ interface, which is taken as an adjustable parameter. From x-ray photoelectron spectroscopy measurements⁹ and previous spectroscopic¹⁶ studies it is known to be a small fraction of ΔE_g , the band-gap discontinuity between the two compounds. As mentioned in the Introduction, previous analyses have found that $|\Delta V_a|/\Delta E_g < 0.1$, and, as will be established more precisely in this paper, the main contributions to the VBO's shown in Fig. 1 are due to shear strain.

The strain shifts of the band edges are given (apart from the hydrostatic contribution to ΔV_a) by²⁰

$$\Delta V_g = 2a(S_{11} + 2S_{12})\epsilon_{\parallel w}/(S_{11} + S_{12}), \quad (3)$$

$$\Delta V_h = +b(S_{11} - S_{12})\epsilon_{\parallel w}/(S_{11} + S_{12}), \quad (4)$$

$$\Delta V_l = -b(S_{11} - S_{12})\epsilon_{\parallel b}/(S_{11} + S_{12}), \quad (5)$$

where $\epsilon_{\parallel w}$ and $\epsilon_{\parallel b}$ are the in-plane strains in the well and in the barrier: $\epsilon_{\parallel i} = a_{\text{substrate}}/a_i - 1$ ($i = w, b$; a_i is the unit cell size), the S_{ij} are the elastic compliance coefficients of CdTe,²¹ and a and b the deformation potentials. In principle there is also a contribution to ΔV_a from the difference of a_v between the well and barrier, but this is negligible because x is small. For the $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ layers we obtain S_{ij} , a , and b by linear interpolation between

their values in CdTe and ZnTe. The deformation potentials are taken as $a = -3.85$ eV,²² $b = -1.15$ eV for CdTe,^{11,23} and $a = -5.48$ eV, $b = -1.3$ eV for ZnTe.²⁴ We have corrected the deformation potentials of CdTe given in Ref. 22, using the elastic constants of Ref. 21. The only one of these parameters whose uncertainty affects the result appreciably is b : the values obtained in the two references are 1.26 and 1.05 eV, respectively, so we assign b an uncertainty of ± 0.1 eV.

$E_c(E_1)$, $E_c(H_1)$, and $E_c(L_1)$ are the lower edges of the lowest subbands calculated using the Kronig-Penney model.^{25,26} The effective masses in the $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ layer are determined by linear interpolation between their values in CdTe and ZnTe.²⁷ One possible source of error is the uncertainty in the hole masses. Cyclotron resonance²⁷ and magneto-optical measurements²⁸ give for the light hole $m_{z1} = 0.128m_0$ and $m_{z1} = 0.159m_0$, respectively (z is the [001] direction). Hermann and Weisbuch²⁹ have given reasons for preferring the cyclotron resonance values.

The only remaining unknown quantities in Eqs. (1) and (2) are the EBE's. Their calculation merits a separate section.

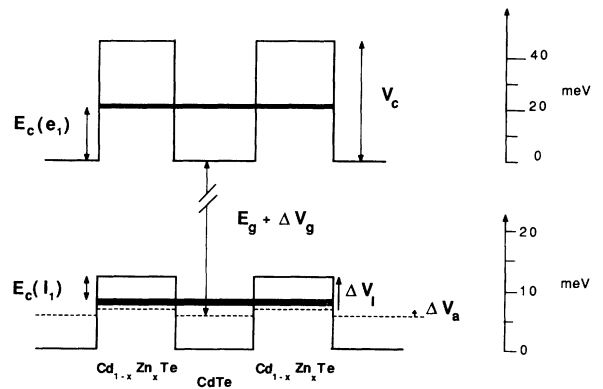


FIG. 1. Type-II light-hole band-gap configuration for sample number 5: c and l refer to the conduction band and to the light-hole valence band, respectively. The dashed line represents the potential in the absence of shear strain: ΔV_a is the average valence-band offset. ΔV_l is the shift of the light-hole band due to shear strain only. The continuous lines show the actual potentials, including the effect of strain, seen by the light hole and by the electron. The shaded areas represent the e_1 and l_1 mini-bands.

CALCULATION OF THE EXCITON BINDING ENERGIES

Since calculation of the EBE in SL's, where miniband effects must be taken into account, is rather involved, we limit ourselves to the case of quantum wells in this paper. The domain of validity of these calculations may be estimated using existing theories for SL's.²

For type-I SL's with equal well and barrier widths, Chomette *et al.*³ have shown that two regimes can be distinguished in the variation of the EBE with the SL period d . For large periods the EBE increase slowly as the period decreases: the exciton is strongly confined in the wells and has approximate two-dimensional (2D) character as in the MQW. At a certain value of d one observes a sudden drop in the EBE followed by a slow decrease toward the bulk value. In this small d regime the exciton is delocalized and has 3D character. The transition between the two regimes takes place when the electron miniband width approaches the Coulomb energy. In the first regime, Dignam and Sipe's calculations² lead to the same values of the EBE for SL's as for QW's.

For type-II SL's the variation of the EBE with the period is completely different. Starting with the 3D value for the equivalent alloy at vanishingly small d , the EBE decreases steadily as d increases and the overlap of the electron and hole wave functions decreases. It has been shown by Dignam and Sipe that for the lowest exciton in a SL the departure from the QW calculation is small and shows up only at very small d . It should be noted that in reality, for very long periods, the exciton tends to be associated with one interface and the electron-hole separation ceases to increase with well width. However, we have performed the calculation (see below) and found that the

$$V_{\text{eff}}(z_v) = V_v(z_v) + \frac{\hbar^2}{2\mu\lambda^2} - \frac{2e^2}{4\pi^2\epsilon\lambda^2} \int_{-\infty}^{+\infty} dz_c \psi_c^2(z_c) \int_0^{+\infty} d\rho \frac{2\pi\rho e^{-2\rho/\lambda}}{[(\rho^2 + (z_c - z_v)^2)^{1/2}]}. \quad (7)$$

Note that the electron wave function is assumed rigid in this calculation. This approximation is the one-dimensional analog of the HTL (Hopfield-Thomas-Logan) model of the exciton bound to an isoelectronic trap,³² generalized to allow for the finite spatial extent of the electron wave function. This generalized HTL model has recently been shown to work remarkably well in the 3D case even when the electron is only weakly bound to the trap.³³

The hole confinement energy is obtained by numerically solving the Schrödinger equation for $\Psi_v(z_v)$. The exciton energy is then obtained by minimizing this energy with respect to the variational parameter λ . The binding energy is the difference between the hole energy calculated with and without Coulomb interaction (see Fig. 2). In the case of the light hole, V_{eff} is the two-well potential shown in Fig. 2: the maximum binding energy is obtained with a hole wave function $\Psi_l(z_l)$ of even parity.

COMPARISON WITH EXPERIMENT

The calculated heavy-hole EBE is virtually independent of the average band offset ΔV_a : over the range

effect on the EBE for our parameters is very small.

In order to calculate the EBE in the QW, we use a variational method, and the diagonal approximation for the excitonic Hamiltonian H :³⁰

$$H = \frac{p_{cz}^2}{2m_c^*} + \frac{p_{vz}^2}{2m_v^*} + \frac{p_{\parallel}^2}{2\mu_{\parallel}} - \frac{e^2}{4\pi\epsilon[(z_c - z_v)^2 + \rho^2]^{1/2}} + V_c(z_c) + V_v(z_v), \quad (6)$$

where c and v refer to the conduction and valence band, respectively [$v = h$ (l) for heavy (light) hole]. Subscript z means "along z (i.e., growth) axis" and \parallel means "in plane (perpendicular to the growth axis)." The electron, hole, and in-plane reduced effective masses are m_c^* , m_v^* , and μ_{\parallel} ($= [m_c^{*-1} + m_v^{*-1}]^{-1}$), z_c , z_v , and ρ ($= \rho_c - \rho_v$) are the corresponding coordinates, and p_{cz} , p_{vz} , and p are the corresponding momentum operators. Thus $[(z_c - z_v)^2 + \rho^2]^{1/2}$ is the electron-hole separation. $V_c(z_c)$ and $V_v(z_v)$ are the band offsets in the conduction and the valence band, respectively, and ϵ is the dielectric constant [we take $\epsilon = 10.6\epsilon_0$ for CdTe (Ref. 31)].

The trial wave function we use is taken in the form $\psi_c(z_c)\Psi_v(z_v)(2/\pi\lambda^2)^{1/2}e^{-\rho/\lambda}$, where λ is a variational parameter representing the in-plane electron-hole separation. $\psi_c(z_c)$ is the usual envelope function which describes the electron motion in its ground state for a QW with finite barrier height. $(2/\pi\lambda^2)^{1/2}e^{-\rho/\lambda}$ is the normalized $1s$ envelope wave function of a 2D hydrogenlike exciton $\Psi_v(z_v)$, describing the motion of the hole in an effective potential V_{eff} , which is the sum of the QW potential $V_v(z_v)$ and the Coulomb interaction with the electron:

$-0.08 < \Delta V_a/x < +0.04$ eV, it varies by less than 3%, which is not significant considering the uncertainty in the other parameters involved in the calculation. On the other hand, it depends strongly on the in-plane hole effective mass $m_{\parallel v}^*$. Valence-band mixing is known to increase $m_{\parallel v}^*$ from its bulk value for the $H1$ and $L1$ confined lev-

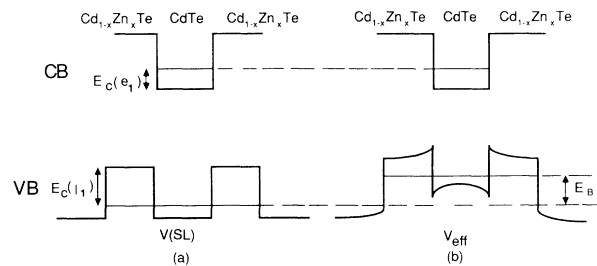


FIG. 2. Type-II configuration (a) without and (b) with Coulomb interaction. We assume that the electron wave function is not affected by presence of the hole, so that the exciton binding energy (EBE) is given by the difference between the confinement energies of the hole calculated in the two situations.

els in other quantum well systems, and preliminary calculations show that this is the case in our structures.³⁴ For this reason we have used two different values of $m_{\parallel v}^*$: the bulk value $m_{\parallel v}^* = (\gamma_1 \pm \gamma_2)^{-1}$ (+ for heavy hole and - for light hole), and $m_{\parallel v}^* = \infty$. Here γ_1 and γ_2 are the Luttinger parameters, for which we took the values $\gamma_1 = 4.11$ and $\gamma_2 = 1.08$ given by Neumann, Nöthe, and Lipari.²⁸ As pointed out above, Le Si Dang, Neu, and Romestain²⁷ give somewhat different values: $\gamma_1 = 4.6$ and $\gamma_2 = 1.6$.

Figure 3 shows our theoretical binding energies for the heavy-hole exciton [Fig. 3(b)] and the light-hole exciton [Fig. 3(a)]. The dotted lines indicate the region of short period SL where our single QW approximation is expected to become inaccurate because of miniband effects. Our double QW approximation (see Fig. 2) for the light-hole exciton includes the miniband effect to a certain extent, so it is quite good even for short period SL, as shown in Ref. 2. The single well model for the heavy-hole exciton is, of course, less good. In each case the lower curve is for $m_{\parallel v}^* = (\gamma_1 \pm \gamma_2)^{-1}$ and the upper for $m_{\parallel v}^* = \infty$, and in the absence of miniband effects the EBE should be bracketed by those two curves. We note the relative insensitivity of the light-hole EBE to $m_{\parallel v}^*$.

For very long SL periods, it is likely that deviations from perfect inversion symmetry, perhaps due to a surface electric field or to differences between the two interfaces, will cause the exciton to be attached to one interface or the other rather than being symmetric in the well. In this case the light-hole EBE will no longer decrease

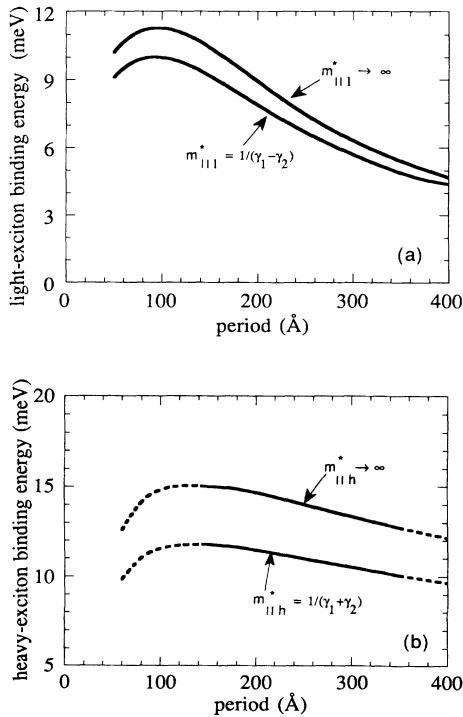


FIG. 3. Calculated EBE as a function of SL period. The lower curve assumes an in-plane hole effective mass $m_{\parallel v}^* = (\gamma_1 \pm \gamma_2)^{-1}$ (+ for heavy and - for light hole) and the upper curve assumes $m_{\parallel v}^* = \infty$. (a) Light-hole exciton; (b) heavy-hole exciton.

with increasing period. An order of magnitude estimate of the polarizability of the exciton in the z direction suggests that for a field of 1 kV cm^{-1} (as would result from a surface charge of order $10^{10} \text{ e cm}^{-2}$) this leveling off will occur at a period of about 400 \AA , corresponding to an EBE of about 4 meV .

Table II compares the theoretically predicted heavy-hole exciton energies with those observed, for samples of different period. As pointed out above, these results are insensitive to the average band offset, which has been taken to be $0.02x \text{ eV}$. The second and third columns show the predictions for the two in-plane hole masses: the values in parentheses are uncertain because of the miniband effects referred to above. Except for these two cases, all the experimental values fall within the range predicted, and indicate that the effective in-plane hole mass is between the two extremes assumed.

Figure 4 shows, as a function of period, the difference between the observed light-hole exciton energies and those predicted, assuming four different values of the average offset. Since, as can be seen from Fig. 3, the theoretical values are rather insensitive to the in-plane hole mass $m_{\parallel v}^*$, this has been taken to have its bulk value $(\gamma_1 - \gamma_2)^{-1}$.

This figure shows very clearly that the best fit is obtained with $\Delta V_a/x = 0.013 \text{ eV}$. If a different value of $m_{\parallel v}^*$ were taken, the fitted value of $\Delta V_a/x$ would be different: for example, if we take $m_{\parallel v}^* = \infty$ we can fit the data with $\Delta V_a/x = 0.07 \text{ eV}$, but the fit is not as good as it is for $m_{\parallel v}^* = (\gamma_1 - \gamma_2)^{-1}$. We estimate the overall fitting error in $\Delta V_a/x$, including uncertainties in the deformation potentials, in the effective masses, and in the EBE calculation, to be $\pm 0.030 \text{ eV}$. We conclude that $-0.017 < \Delta V_a/x < +0.043 \text{ eV}$. Thus it appears that within our experimental accuracy the average VBO is indeed zero in this system.

Our final task is to compare this value of $\Delta V_a/x$ with the predicted values. Bertho *et al.*¹⁶ calculate $\Delta V_a/x = 0.128 \text{ eV}$. van de Walle¹⁵ calculates the chemical offset ΔV_v and the hydrostatic-strain contribution separately. We may write

$$\Delta V_a = \Delta V_v - 2a_v(S_{11} + 2S_{12})(\epsilon_{\parallel b} - \epsilon_{\parallel w}) / (S_{11} + S_{12}). \quad (8)$$

In this expression we have assumed that the compliance coefficients and the deformation potentials in both the well and the barrier have the values for the equivalent

TABLE II. Comparison of theoretical and observed positions of the heavy-hole exciton transition, for two different choices of the in-plane mass $m_{\parallel v}^*$.

Sample number	Period (Å)	Expt.	$E(e_1 h_1)$ $1/(\gamma_1 + \gamma_2)$ (meV)	∞
3	278	1601.7	1604.2	1601.6
5	254	1603.3	1605.9	1603.1
6	209	1613.0	1614.5	1611.6
1	144	1612.0	1614.4	1611.4
4	121	1615.0	(1614.0)	(1611.0)
2	67	1618.75	(1617.5)	(1615.2)

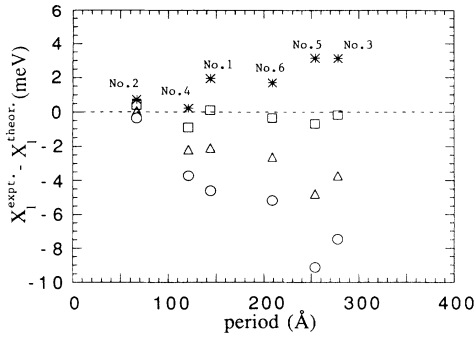


FIG. 4. Difference between calculated and observed energy of the light-hole exciton transition, as a function of SL period. The assumed in-plane mass is $m_{||v}^* = (\gamma_1 - \gamma_2)^{-1}$. The fitting parameter $\Delta V_a/x$ takes the following values (in eV): stars -0.042 , squares $+0.013$, triangles $+0.069$, circles $+0.123$. The fit clearly favors the value $+0.013$ eV.

4% alloy. This is a good approximation in these strain compensated superlattices grown pseudomorphically on a $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ substrate with $y=0.04$.

van de Walle's calculations give $a_v=0.55$ eV for CdTe and 0.79 for ZnTe, whence linear interpolation gives $a_v=0.56$ eV for 4% average material, so that the strain term is $-0.024x$ eV. The calculations give $\Delta V_v/x=0.11$ eV (including the correction for the difference in spin-orbit coupling) so that his predicted value of $\Delta V_a/x$ is 0.09 eV. Tersoff,¹⁴ on the other hand, gives $\Delta V_v/x=-0.01$ eV. If we combine this with van de Walle's value of a_v we obtain a predicted value of $\Delta V_a/x=-0.03$ eV. Our experimental result of 0.013 ± 0.03 eV thus lies between the theoretical estimates, but is closer to Tersoff's, and is not really consistent with any of them.

It is common in the literature to follow Camphausen, Connel, and Paul³⁵ in taking $a_v = -a/3$, so that $a_v = 1.28$ eV and the second term in Eq. (8) becomes $-0.054x$ eV. Combining this with van de Walle's value of ΔV_v would improve the agreement between theory and experiment, but we see no justification for this procedure, nor any *a priori* reason to prefer Camphausen's older theoretical value of a_v over that of van de Walle.

CONCLUSION

$\text{CdTe}/\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ SL's allow us to study spatially direct and indirect exciton transitions over a large range of SL period. We have compared our experimental results with a simple theoretical model in which the binding energies of both direct and indirect excitons were calculated. A detailed fit to our experimental results, taking into account the uncertainty in the parameters used, shows that the average VBO is only $(2 \pm 4)\%$ of the band-gap difference between CdTe and $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ for $x \approx 0.08$. Comparison with theoretical estimates shows that there is a partial cancellation between the chemical and hydrostatic-strain components of the VBO, but that both are small. Our result confirms that uniaxial strain is predominantly responsible for the VBO (Fig. 1) and hence for the type-II character of the light-hole exciton.

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