Heavy-light hole mixing at zinc-blende (001) interfaces under normal incidence

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The reduced point symmetry C_{2v} of a zinc-blende-based (001) interface allows mixing between heavy- and light-hole states even under normal incidence. We have generalized the envelope function approximation to take into account such a mixing by including off-diagonal terms into boundary conditions for the envelopes. The normal off-diagonal hole reflection from a GaAs/AlAs(001) heterointerface as well as Γ-point interband matrix elements in GaAs/AlAs multilayered structures have been calculated and the results have been compared with those obtained by pseudopotential and tight-binding calculations. The best fit with the numerical calculations gives for the dimensionless heavy-light hole mixing coefficient values $t_{l\text{-}h}=0.9$ and 0.32. The theory of exchange splitting of excitonic levels in type II GaAs/AlAs superlattices has been extended to include not only the heavy-light hole mixing but also an admixture of spin-orbit-split states in the heavy-hole wave function. An agreement between theory and experiment for the anisotropic exchange splitting has been achieved for $t_{l\text{-}h}=0.5$. A tight-binding model has been used to relate the microscopic parameters with coefficients in the boundary conditions for the hole envelope function. The tight-binding model estimation of $t_{l\text{-}h}=0.44$ is in reasonable agreement with the other estimations of $t_{l\text{-}h}$. [S0163-1829(96)09031-5]

I. INTRODUCTION

Quantum-mechanically, the most pronounced effects of band offsets at semiconductor heterointerfaces are the confinement of free carriers in quantum-well (QW) structures and redistribution of the electron probability density between adjacent layers in superlattices (SL). Since the interfaces reduce the translational and point symmetries of the system, they can lead not only to mixing between electronic states from the same band but also to intervalley and interband or intersubband mixings. In zinc-blende-based heterostructures grown along the [001] crystallographic axis the lack of microscopic translational symmetry can result in remarkable coupling between Γ and X_z valley states as well as between the indirect X_x and X_y valley states.[1–3] Within the envelope function approximation (EFA), which makes use of the bulk symmetry of the $\mathbf{k}$ vector in the growth direction, the mixing between heavy-hole (hh) and light-hole (lh) states is well described for oblique incidence on an interface, i.e., for a nonzero in-plane wave vector $\mathbf{k}_{\rm in}$ (see, e.g., Refs. 4 and 5), or at normal incidence on interfaces grown along directions with the higher Miller indices, say along the [110] or [113] directions.[6,7] For (001)-grown structures, however, it is generally accepted that when using the EFA this mixing is forbidden for normally incident holes.[8–10] This is in contrast with the fact that according to the point symmetry C_{2v} of an ideal GaAs/AlAs(001) interface hh and lh states transform according to equivalent spinor representations and hence the interface-induced hh-lh coupling is allowed.

In Refs. 11 and 12 we postulated this mixing by adding additional terms in the boundary conditions for the hole envelope function at interfaces in order to explain the nature of the giant anisotropic exchange splitting of excitonic levels observed in type II GaAs/AlAs SLs.[13,14] Recent numerical calculations[15] performed by using the empirical pseudopotential formalism have shown that a heavy hole reflected under normal incidence from a single GaAs/AlAs(001) heterojunction contains a considerable light-hole amplitude. It should be mentioned that earlier Schulman and Chang[16] solved the tight-binding model and reported the mixing of the heavy- and light-hole states with $\mathbf{k}_{in}=0$ in the (001)-grown GaAs/$Ga_{1-x}Al_xAs$ and InAs/GaSb multilayered heterostructures. Nevertheless in the later EFA calculations Zhu and Huang[8] and Chu and Chang[17] assumed fourfold or even axial symmetries which forbid the normal-incidence heavy-light-hole mixing.

In the present work the EFA is extended to describe the normal-incidence heavy-light-hole mixing and fill a gap between the conventional EFA approach and numerical pseudopotential or tight-binding calculations. In Sec. II we analyze the boundary conditions for the envelope functions by using the C_{2v} symmetry of the (001) interface to demonstrate unambiguously the possibility of hh-lh coupling for vanishing in-plane wave vector. Using this model in Sec. III we calculate the hole reflection coefficients and compare them with values obtained from empirical pseudopotential calculations of Ref. 15. In Sec. IV we generalize the theory of anisotropic exchange splitting of excitonic levels in type II GaAs/AlAs superlattices to take into account an admixture of spin-orbit-split states in the heavy-hole wave function. In Sec. V we show by calculating optical interband matrix elements that, due to the hh-lh mixing, transitions between subband pairs of opposite parity become allowed, as in tight-binding calculations.[16] In Sec. VI we establish a relation between microscopic parameters of the tight-binding model and the coefficient describing the hh-lh hole mixing in the boundary conditions.

II. SYMMETRY CONSIDERATIONS

The Bloch functions at the valence band maximum of a semiconductor with the point symmetry T_d can be formulated as $|X\uparrow\rangle$, $|Y\uparrow\rangle$, $|Z\uparrow\rangle$, $|X\downarrow\rangle$, $|Y\downarrow\rangle$, $|Z\downarrow\rangle$ (set 1: $|1,i\rangle$, $i=1,\ldots,6$) or as $|\Gamma_8,3/2\rangle$, $|\Gamma_8,1/2\rangle$, $|\Gamma_8,-1/2\rangle$, $|\Gamma_8,-3/2\rangle$, $|\Gamma_7,1/2\rangle$, $|\Gamma_7,-1/2\rangle$ (set 2: $|2,l\rangle$, $l=1,\ldots,6$) where the coordinate system $x\|[100],y\|[010],z\|[001]$ is assumed. These sets transform according to the direct product $\Gamma_6\times\Gamma_5$ or its decomposition $\Gamma_8+\Gamma_7$, respectively. The hole wave function in a quantum structure can be expanded in either set

$$\psi=\sum_{i=1}^{6} F_i(\mathbf{r})|1,i\rangle=\sum_{l=1}^{6}\Phi_l(\mathbf{r})|2,l\rangle \tag{1}$$

with envelope functions F_i or Φ_l depending only on the coordinate z if we describe hh-lh mixing under normal incidence.

In the absence of spin-orbit splitting of the valence band the simplest boundary conditions for the envelopes $F_i(z)$ are

$$\mathbf{F}_A=\mathbf{F}_B,\qquad (\hat{v}_z\mathbf{F})_A=(\hat{v}_z\mathbf{F})_B, \tag{2}$$

where $\mathbf{F}$ is the column with the components F_i, the subscripts A,B indicate the compositional material, say GaAs or AlAs, and $\hat{v}_z$ is the normal component of the hole velocity operator

$$\hat{v}_z=\frac{1}{\hbar}\frac{\partial H}{\partial k_z}. \tag{3}$$

For normal incidence ($\mathbf{k}_{\rm in}=0$) the effective hole Hamiltonian is

$$H=\begin{bmatrix} H_{\Gamma_5} & 0 \\ 0 & H_{\Gamma_5}\end{bmatrix} \tag{4}$$

with $H_{\Gamma_5}=[L-(L-M)I_z^2]\hat{k}_z^2$ $\hat{k}_z=-i\partial/\partial z$, band parameters L, M, and the 3×3 matrix I_z of the angular momentum $I=1$ so that

$$I_z^2=\begin{bmatrix}1&0&0\\0&1&0\\0&0&0\end{bmatrix}.$$

The hh-lh mixing, or mixing between X and Y orbital states, which is possible due to the C_{2v} symmetry of a (001) interface (see Fig. 1), can be described by adding to H of Eq. (4) a coupling Hamiltonian

$$H_{X\text{-}Y}=\pm\frac{\hbar^2 t_{X-Y}}{m_0 a_0}\begin{bmatrix}\{I_xI_y\}&0\\0&\{I_xI_y\}\end{bmatrix}\delta(z-z_i). \tag{5}$$

The essential features are the symmetrized product

$$\{I_xI_y\}\equiv\frac{1}{2}(I_xI_y+I_yI_x)=\frac{1}{2}\begin{bmatrix}0&-1&0\\-1&0&0\\0&0&0\end{bmatrix}$$

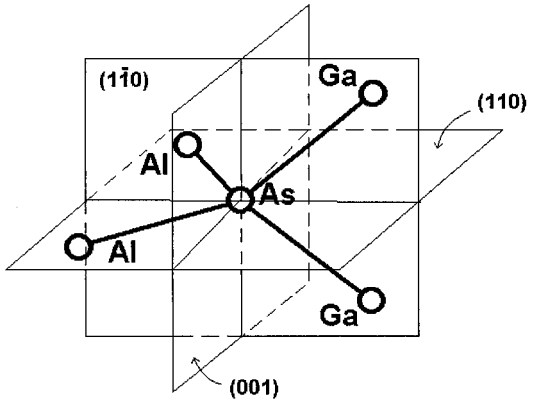

FIG. 1. The nearest neighbors of an As interface atom. The point symmetry C_{2v} of a single heterojunction contains the twofold rotation axis C_2 parallel to the growth direction [001] and two mirror planes (110) and ($1\bar{1}0$).

which is an invariant under C_{2v} and the δ-function with z_i being the coordinate of the interface. The sign $\pm$ refers to BA or AB interfaces and the prefactor with Planck's constant $\hbar$, free electron mass m_0, and lattice constant a_0 (assumed to be the same for A and B) has been introduced to characterize the X-Y mixing by the dimensionless real parameter $t_{X\text{-}Y}$. Taking into account $H_{X\text{-}Y}$ the boundary conditions have to be changed by adding the term

$$\mathbf{f}=i\frac{\hbar t_{X\text{-}Y}}{a_0 m_0}\begin{bmatrix}2\{I_xI_y\}&0\\0&2\{I_xI_y\}\end{bmatrix}\mathbf{F} \tag{6}$$

to $(\hat{v}_z\mathbf{F})_B$ on the right-hand side of Eq. (2). Note that $\{I_xI_y\}$ has the same transformation properties as $\hat{v}_z$. We remind the reader that the C_{2v} point group consists of the rotation axis $C_2\|z$ and two mirror planes (110) and ($1\bar{1}0$) (Fig. 1).

Including the spin-orbit interaction $-\frac{2}{3}\Delta_{\rm so}(\mathbf{sI})$ the boundary conditions are obtained by applying the unitary transformation ''set 1 $\rightarrow$ set 2'' to Eq. (2) and to the mixing term (6):

$$\Phi_A=\Phi_B,\qquad (\hat{v}_z\Phi)_A=(\hat{v}_z\Phi)_B-\frac{2}{3}i\frac{\hbar}{a_0 m_0}t_{X\text{-}Y}R\Phi. \tag{7}$$

Here the velocity operator $\hat{v}_z$ is connected by Eq. (3) with the 6×6 $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian in the basis set $|2,l\rangle$ (see Ref. 18) and R is the 6×6 matrix

$$R=\begin{bmatrix}\{J_xJ_y\}&3U_{xy}\\3U_{xy}^{+}&0\end{bmatrix} \tag{8}$$

composed of angular momentum matrices J_α for $J=3/2$ and the 4×2 intersubband matrix U_{xy} introduced in Ref. 18 (see also Ref. 19).

If the hole energy E is small compared with the spin-orbit splitting $\Delta_{\rm so}$, then, for $M/L\ll1$, the mixing between the Γ_8 and Γ_7 subspaces can be neglected and we retain in Eq. (7) only the first four components Φ_j and in R the 4×4

block $\{J_xJ_y\}$. In this case the boundary conditions coincide with those proposed in Refs. 11 and 12,

$$(\Phi_j)_A=(\Phi_j)_B,$$

$$(\nabla^j\Phi_j)_A=(\nabla^j\Phi_j)_B+\frac{2}{\sqrt{3}}t_{l\text{-}h}\{J_xJ_y\}_{jj'}\Phi_{j'} \tag{9}$$

if we put

$$t_{l\text{-}h}=\frac{1}{\sqrt{3}}t_{X\text{-}Y}. \tag{10}$$

Here

$$\nabla^{\pm 3/2}=a_0\frac{m_0}{m_{\rm hh}}\frac{\partial}{\partial z},\quad \nabla^{\pm 1/2}=a_0\frac{m_0}{m_{\rm lh}}\frac{\partial}{\partial z}$$

and we use the notations $m^A_{\rm hh}$, $m^B_{\rm hh}$, $m^A_{\rm lh}$, and $m^B_{\rm lh}$ for the effective masses of heavy and light holes in the A and B layers.

III. NORMAL HEAVY-LIGHT HOLE REFLECTION FROM GaAs/AlAs (001) INTERFACE

Consider now a free hole normally incident on a GaAs/AlAs interface. Its energy is chosen to be smaller than the GaAs spin-orbit splitting $\Delta_{\rm so}\approx 0.3$ eV which is also smaller than the valence-band offset $V_0\approx 0.5$ eV. In this case HH and LH states on the GaAs side are propagating, while spin-split-off states in GaAs and all hole states on the AlAs side are evanescent. On the GaAs side the first four envelopes Φ_l in Eq. (1) can be written as a sum of two columns:

$$\Phi_{\rm in}=\begin{bmatrix} e^{ik_hz}\varphi^0_{3/2}\\ e^{ik_lz}\varphi^0_{1/2}\\ e^{ik_lz}\varphi^0_{-1/2}\\ e^{ik_hz}\varphi^0_{-3/2}\end{bmatrix},\quad \Phi_{\rm out}=\begin{bmatrix} e^{-ik_hz}\varphi^r_{3/2}\\ e^{-ik_lz}\varphi^r_{1/2}\\ e^{-ik_lz}\varphi^r_{-1/2}\\ e^{-ik_hz}\varphi^r_{-3/2}\end{bmatrix},$$

representing, respectively, the incident and reflected waves. Here

$$k_h=(2m^A_{\rm hh}E/\hbar^2)^{1/2},\quad k_l=(2m^A_{\rm lh}E/\hbar^2)^{1/2}=(m^A_{\rm lh}/m^A_{\rm hh})^{1/2}k_h. \tag{11}$$

Due to the intersubband mixing at the interface (as described in Sec. II) the off-diagonal heavy-light and light-heavy reflection coefficients, $\rho_{l,h}$ and $\rho_{h,l}$, are nonzero and the particle-flux conservation law imposes the following relations between the diagonal and off-diagonal reflectivities:

$$\rho_{h,h}+\rho_{l,h}=\rho_{l,l}+\rho_{h,l}=1.$$

On the other hand, the time inversion symmetry leads to the relation $\rho_{l,h}=\rho_{h,l}\equiv\rho$. This allows us to present the 4×4 matrix that relates φ^r_l and φ^0_l in the general form

$$\tilde{\varphi}^{\,r}=-\left[\sqrt{1-\rho}(e^{i\delta_h}M_h+e^{i\delta_l}M_l)+\sqrt{\rho}\frac{2i}{\sqrt{3}}e^{i\tilde{\delta}}\{J_xJ_y\}\right]\tilde{\varphi}^0. \tag{12}$$

Here $\rho\equiv\rho_{l,h}$, $\tilde{\varphi}^{\,r}$ and $\tilde{\varphi}^0$ are four-component columns connected with φ^r and φ^0 by

$$\tilde{\varphi}^0_j=\left(\frac{m_0}{m_j}\right)^{1/4}\varphi^0_j,\tilde{\varphi}^{\,r}_j=\left(\frac{m_0}{m_j}\right)^{1/4}\varphi^r_j, \tag{13}$$

$m_j=m^A_{\rm hh}$ for $j=\pm 3/2$ and $m_j=m^A_{\rm lh}$ for $j=\pm 1/2$,

$$M_h=\frac{1}{2}\left(J_z^2-\frac{1}{4}\right),\quad M_l=1-M_h=\frac{1}{2}\left(\frac{9}{4}-J_z^2\right).$$

The further simplifications follow if we assume the incident energy is much smaller than Δ_{so} and $M/L\ll 1$, in which case the spin-split-off states can be excluded from consideration at all and one can use the Luttinger 4×4 Hamiltonian together with the boundary conditions in the form of Eq. (9). The latter may be rewritten in terms of the φ^0_l and φ^r_l amplitudes as

$$\tau^*_h\varphi^0_{\pm 3/2}=-\tau_h\varphi^r_{\pm 3/2}\mp t_{l\text{-}h}(\varphi^0_{\mp 1/2}+\varphi^r_{\mp 1/2}),$$
$$\tau^*_l\varphi^0_{\pm 1/2}=-\tau_l\varphi^r_{\pm 1/2}\mp t_{l\text{-}h}(\varphi^0_{\mp 3/2}+\varphi^r_{\mp 3/2}), \tag{14}$$

where

$$\tau_h=a_0m_0\left(\frac{\kappa_h}{m^B_{\rm hh}}-i\frac{k_h}{m^A_{\rm hh}}\right),\quad \tau_l=a_0m_0\left(\frac{\kappa_l}{m^B_{\rm lh}}-i\frac{k_l}{m^A_{\rm lh}}\right) \tag{15}$$

and

$$\kappa_h=[2m^B_{\rm hh}(V_0-E)/\hbar^2]^{1/2},\quad \kappa_l=[2m^B_{\rm lh}(V_0-E)/\hbar^2]^{1/2}. \tag{16}$$

One can see that in accordance with the C_{2v} point symmetry the mixing occurs between the hole spin states $+3/2$ and $-1/2$ or $-3/2$ and $+1/2$. Equation (14) can be readily solved resulting in

$$\rho=4t^2_{l\text{-}h}\frac{m_0^2}{m^A_{\rm hh}m^A_{\rm lh}}\frac{k_hk_la_0^2}{|\tau_h\tau_l-t^2_{l\text{-}h}|^2}. \tag{17}$$

Taking into account that the term $t^2_{l\text{-}h}$ in the denominator is small as compared with $\tau_h\tau_l$ we finally arrive at

$$\rho\approx 2t^2_{l\text{-}h}\frac{m^B_{\rm hh}m^B_{\rm lh}}{\sqrt{m^A_{\rm hh}m^A_{\rm lh}}}\frac{\hbar^2}{a_0^2m_0^2}\frac{E}{V_0^2}. \tag{18}$$

In the same approximation the phases in Eq. (12) are given by

$$\delta_h=\arg\left(\frac{\tau^*_h\tau_l-t^2_{l\text{-}h}}{\tau_h\tau_l-t^2_{l\text{-}h}}\right)\approx-\arg\tau^2_h,\quad \delta_l\approx-\arg\tau^2_l,$$
$$\tilde{\delta}\approx-\arg(\tau_h\tau_l). \tag{19}$$

Thus, for small hole kinetic energies ($E\ll\Delta_{\rm so}$) the off-diagonal reflectivity is a linear function of E.

The energy dependence $\rho(E)$ is shown in Fig. 2. The straight dashed line represents the approximate result given by Eq. (18). The triangles reproduce the empirical pseudopotential results of Edwards and Inkson.[15] The solid curve is calculated in the $\Gamma_8+\Gamma_7$ band model with the boundary conditions (7) for the following values of band parameters:

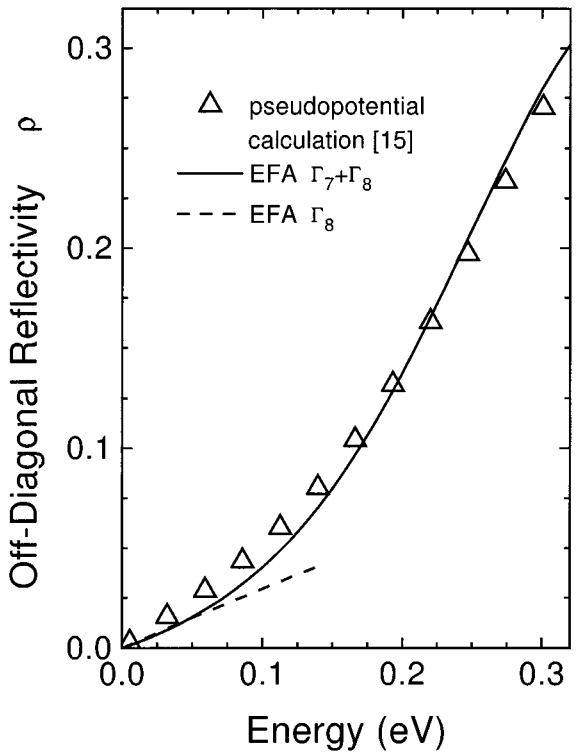

FIG. 2. The heavy-light hole off-diagonal reflectivity versus the energy E of a hole normally incident on a GaAs/AlAs single heterointerface from the GaAs side. Solid curve is calculated in the generalized EFA by using the following set of parameters: $m_{\rm hh}=0.45m_0$, $m_{\rm lh}=0.09m_0$, $V_0=0.53$ eV, $\Delta_{\rm so}=0.35$ eV, and $t_{l\text{-}h}=0.9$ (or $t_{X\text{-}Y}=1.5$), dashed line represents the approximate result of Eq. (18), and triangles show the result of pseudopotential model calculations (Ref. 15).

$V_0/\Delta E_g=0.4$, $m^A_{\rm hh}=m^B_{\rm hh}\equiv m_{\rm hh}=0.45\ m_0$, $m^A_{\rm lh}=m^B_{\rm lh}\equiv m_{\rm lh}=0.09\ m_0$, $t_{X-Y}\equiv\sqrt{3}t_{l\text{-}h}=1.5$, where ΔE_g is the difference between band gaps in AlAs and GaAs. As follows from Sec. II the heavy-light hole mixing for $k_x=k_y=0$ is directly connected with interface-induced coupling between X and Y orbital states and has a nonrelativistic origin. Estimates show that the mixing due to relativistic effects such as linear-in-k_z terms in the hole effective Hamiltonian (see, e.g., Ref. 20) is too weak in comparison with the nonrelativistic mixing and can be neglected. In Ref. 15 the authors question the validity of the effective mass theory or Luttinger Hamiltonian approach. Now the answer is that this approach is valid if one includes terms like Eq. (5) or Eq. (6) which follow from the point symmetry of the interface and account for the intersubband mixing.

Kiledjian *et al.*[21] used a ten-band tight-binding model to calculate the tunneling of holes in a double-barrier GaAs/Ga_xAl_{1-x}As heterostructure. They report a significant mixing effect between heavy- and light-hole states even for zero in-plane wave-vector component. Obviously this effect can be also described in the frame of the effective mass approximation with the generalized boundary conditions.

IV. ANISOTROPIC EXCHANGE SPLITTING OF EXCITONIC LEVELS IN TYPE II GaAs/AlAs(001) SLs

In an ideal GaAs/AlAs SL grown along the [001] direction, the $1s$ heavy-hole exciton level is split into a radiative doublet and two close-lying nonradiative sublevels. However, it was found experimentally[13,14,22–25] that, for localized excitons in type II GaAs/AlAs(001) SLs, the degeneracy of the radiative states is lifted and the two sublevels are dipole-active in the $[110]$ and $[1\bar{1}0]$ directions. Moreover, it was established[13] that in the same sample there exist simultaneously two classes of excitons with equal absolute values but opposite signs of the difference Δ between the dipole-active sublevels $\varepsilon_{[110]}$ and $\varepsilon_{[1\bar{1}0]}$. The exchange-interaction anisotropy was related in Refs. 11 and 12 to the heavy-light hole mixing described by the additional term in Eq. (9). Then the pair of wave functions at the bottom of the lowest heavy-hole subband hh1 can be written as

$$\varphi^{(\rm hh1)}_{\pm 3/2}(z)=C(z)|\Gamma_8,\pm 3/2\rangle \pm iS(z)|\Gamma_8,\mp 1/2\rangle, \quad (20)$$

where real envelope functions $C(z)$ and $S(z)$ are, respectively, even and odd with respect to the reflection $z\rightarrow -z$ for the origin $z=0$ taken in the center of a GaAs well.

Excitons contributing to the low-temperature photoluminescence of undoped type II SLs are two-particle excitations localized by the structure imperfections in the plane of interfaces with an X-electron and a Γ-hole confined inside two neighboring AlAs and GaAs layers. This presupposes an existence of two classes of localized excitons with a left- and right-hand-side electron. Let the localization length exceed the exciton Bohr radius a_B, describing the in-plane relative motion of the electron-hole pair. Then, for both classes, the anisotropic exchange splitting, $\Delta=\varepsilon_{[110]}-\varepsilon_{[1\bar{1}0]}$, is given by[12]

$$\Delta_{L,R}=\frac{16a_0^3}{\sqrt{3}\pi a_B^2}\varepsilon_0\int C(z)S(z)[u^2_{L,R}(z)+v^2_{L,R}(z)]dz, \quad (21)$$

where $u_{L,R}(z)$ and $v_{L,R}(z)$ are the X_1 and X_3 envelopes of an X-electron confined, respectively, in the left- and right-hand AlAs layers and ε_0 determines the initial electron-hole exchange interaction taken in the form

$$V_{\rm exch}=-\varepsilon_0 a_0^3\delta(\mathbf{r}_e-\mathbf{r}_h)\boldsymbol{\sigma}_e\boldsymbol{\sigma}_h,$$

where $\sigma_{e\alpha},\sigma_{h\alpha}$ are the electron and hole spin Pauli matrices. Taking into account that $u_L(z)=u_R(-z)$, $C(z)$ is even, and $S(z)$ is odd, one immediately obtains $\Delta_L=-\Delta_R$, which explains the two classes of excitons observed experimentally. The best fit to the experimental data was achieved for the value $t_{l\text{-}h}\cong 1.4$.

In the present work we have extended the theory[12] to take the split-off band Γ_7 into consideration, in which case the function $\varphi^{(\rm hh1)}_{\pm 3/2}(z)$ contains three contributions

$$\varphi^{(\rm hh1)}_{\pm 3/2}(z)=C(z)|\Gamma_8,\pm 3/2\rangle \pm iS(z)|\Gamma_8,\mp 1/2\rangle + i\overline{S(z)}|\Gamma_7,\mp 1/2\rangle, \quad (22)$$

where $\overline{S(z)}$ is an odd function of z. As a result, Eq. (21) transforms into

$$\Delta_{L,R}=\frac{16a_0^3}{\sqrt{3}\pi a_B^2}\varepsilon_0\int C(z)[S(z)+\sqrt{2}\overline{S(z)}]\times[u_{L,R}^2(z)+v_{L,R}^2(z)]dz. \quad (23)$$

An agreement with the experimental values of Δ is obtained for a considerably smaller value of the mixing coefficient: $t_{l\text{-}h}=0.5$. Thus, in heterostructures with narrow wells, an admixture of the split-off band plays an important role and cannot be excluded while calculating the anisotropic exchange splitting of the $1s$ heavy-hole exciton level in the type II superlattices.

V. MATRIX ELEMENTS FOR INTERBAND OPTICAL TRANSITIONS IN A QW

The HH-LH mixing modifies interband and intersubband optical matrix elements in QW structures and SLs. Following Chang and Schulman[16] we calculate the momentum matrix element $P_{\mathrm{CB1,VBi}}$ (at $k_x=k_y=0$) between the lowest Γ-conduction subband CB1 and the second and third valence subbands, VB2 and VB3, in GaAs/AlAs QWs. It is known that the second heavy-hole (hh2) and the lowest light-hole (lh1) subbands cross each other at a certain value of the QW width, corresponding to a particular number N_{cr} of GaAs monomolecular layers. For the structures with N near N_{cr} these two states are strongly coupled due to the heavy-light hole mixing at the interfaces and form the hybrids VB2 and VB3. If the mixing is neglected, the envelope functions Φ in Eq. (1) are given in the conventional form

$$\Phi_{\mathrm{hh2}}(z)=\begin{cases} C_h\cos k_h z & \text{if } |z|\leqslant\dfrac{a}{2},\\ C_h\cos\phi_h\exp\left[-\kappa_h\left(|z|-\dfrac{a}{2}\right)\right] & \text{if } |z|\geqslant\dfrac{a}{2},\end{cases}$$

$$\Phi_{\mathrm{lh1}}(z)=\begin{cases} C_l\sin k_l z & \text{if } |z|\leqslant\dfrac{a}{2},\\ \pm C_l\sin\phi_l\exp\left[-\kappa_l\left(|z|-\dfrac{a}{2}\right)\right] & \text{if } |z|\geqslant\dfrac{a}{2},\end{cases}$$

where the normalization coefficients are

$$C_h=\left[\frac{a}{2}\left(1+\frac{\sin k_h a}{k_h a}+\frac{1+\cos k_h a}{2\kappa_h a}\right)\right]^{-1/2},$$

$$C_l=\left[\frac{a}{2}\left(1-\frac{\sin k_l a}{k_l a}+\frac{1-\cos k_l a}{2\kappa_l a}\right)\right]^{-1/2},$$

$\phi_h=k_h a/2$, $\phi_l=k_l a/2$, and k_h, k_l, κ_h, and κ_l are expressed via the confinement energies E_{hh2}^0 and E_{lh1}^0, respectively, by Eq. (11) and Eq. (16). The equations for E_{hh2}^0 and E_{lh1}^0 are standard:

$$\tan\phi_h=\frac{m_{\mathrm{hh}}^A}{m_{\mathrm{hh}}^B}\frac{\kappa_h}{k_h},\quad \cot\phi_l=-\frac{m_{\mathrm{lh}}^A}{m_{\mathrm{lh}}^B}\frac{\kappa_l}{k_l}.$$

Neglecting spin-split-off states we can transform the δ-function contribution (5) into

$$H_{l\text{-}h}=\pm\frac{t_{l\text{-}h}\hbar^2}{\sqrt{3}m_0 a_0}\{J_x J_y\}\delta(z-z_i).$$

Then the coupling matrix element is derived as

$$\langle \mathrm{hh2},\pm 3/2|H_{l\text{-}h}|\mathrm{lh1},\mp 1/2\rangle=\pm i\frac{t_{l\text{-}h}\hbar^2}{m_0 a_0}C_h C_l\cos\phi_h\sin\phi_l. \quad (24)$$

In the two-level approximation, the VB3 and VB2 subband energies are given by

$$E_{\mathrm{VB}i}=\frac{1}{2}(E_{\mathrm{hh2}}^0+E_{\mathrm{lh1}}^0)\pm W, \quad (25)$$

where

$$W=\sqrt{\overline{\Delta}^2+\overline{V}^2},\quad \overline{\Delta}=\frac{1}{2}(E_{\mathrm{hh2}}^0-E_{\mathrm{lh1}}^0)$$

and $\overline{V}$ is the modulus of the coupling matrix element (24). The dependences of $E_{\mathrm{hh2}}^0, E_{\mathrm{lh1}}^0, E_{\mathrm{VB2}}$, and E_{VB3} upon the QW width are shown in Fig. 3(a).

Let $P_{\mathrm{CB1,lh1}}$ label the momentum matrix element for the transitions at the point $k_x=k_y=0$ from the unmixed lh1 states. Since the optical transitions hh2$\rightarrow$CB1 are forbidden, the matrix element $P_{\mathrm{CB1,VB}i}$ is proportional to the admixture of the lh1 state in the VBi hybrid. It follows then that the relative squared matrix element $Q(\mathrm{CB1-VB}i)=|P_{\mathrm{CB1,VB}i}/P_{\mathrm{CB1,lh1}}|^2$ can be written as

$$Q(\mathrm{CB1-VB2})=\frac{W+\overline{\Delta}}{2W},\quad Q(\mathrm{CB1-VB3})=\frac{W-\overline{\Delta}}{2W}. \quad (26)$$

Thus, in the vicinity of the crossing point the sum of $Q(\mathrm{CB1-VB2})$ and $Q(\mathrm{CB1-VB3})$ should be constant and equal to unity. In Fig. 3(b) we show the calculated dependence of $Q(CB1-VBi)$ on the QW width for $m_{\mathrm{hh}}=0.45m_0$, $m_{\mathrm{lh}}=0.09m_0$, $V_0=0.53$ eV, $t_{l\text{-}h}=0.5$. Finally in Fig. 3(c) we compare the tight-binding calculations of Chang and Schulman (squares) with the EFA curves calculated for $V_0=0.15\,\Delta E_g$, $m_{\mathrm{hh}}=0.45$, $m_{\mathrm{lh}}=0.07m_0$, $t_{l\text{-}h}=0.32$. The latter values of V_0 and m_{lh} are chosen in order to obtain the same critical number N_{cr} as in Ref. 16.

Winkler[26] applied a multiband $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian and reproduced the essential details of experimental absorption spectra. However a weak electric field in the growth direction was assumed in order to make CB1$-$hh2($1s$) excitons dipole-allowed and describe the CB1$-$hh2 spectral peak observed by Reynolds *et al.*[28] The above considerations remove the restrictions[8,17] imposed on the selection rules for the exciton angular momentum. In particular, due to the hh2$-$lh1 mixing not only $2p$ but also $1s$ excitons CB1$-$hh2 or CB2$-$lh1 become dipole active and can contribute to the optical spectra[27,28] even in the absence of electric fields.

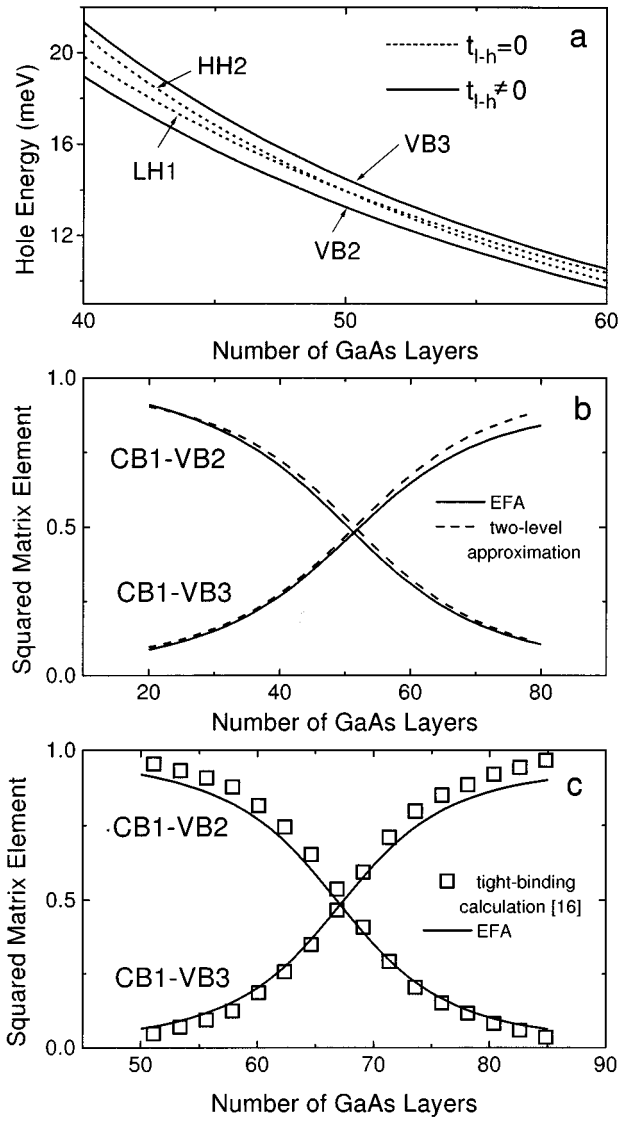

FIG. 3. (a) Anticrossing between the second and third valence subbands in GaAs/AlAs QW structures. Solid and dotted curves are calculated, respectively, for $t_{l\text{-}h}=0.5$ (or $t_{X\text{-}Y}=0.86$) and neglecting the hh-lh mixing described by the additional term in the boundary conditions (9). The valence band offset is taken as $V_0=0.4\Delta E_g$. Other parameters are the same as in Fig. 2. The monomolecular layer thickness is equal to $a_0/2=2.83$ Å. (b) The relative squared matrix elements $Q(\mathrm{CB1}-\mathrm{VB}i)=|P_{\mathrm{CB1,VB}i}/P_{\mathrm{CB1,lh1}}|^2$ as a function of monomolecular layer number in the GaAs layer. Solid curves are calculated in the generalized EFA while dashed curves represent the two-level approximation [see Eq. (26)]. The parameters are the same as in (a). (c) Normalized squared matrix elements for optical transitions VB2,VB3→CB1 (at the point $\mathbf{k}_{\mathrm{in}}=0$) calculated in this work ($m_{\mathrm{hh}}=0.45m_0$, $m_{\mathrm{lh}}=0.07m_0$, $V_0/\Delta E_g=0.15$, $t_{l\text{-}h}=0.4$) and in a nearest-neighbor tight-binding model (Ref. 16) (squares).

VI. HEAVY-LIGHT HOLE MIXING IN THE TIGHT-BINDING MODEL

In order to derive a microscopic expression for the X-Y mixing parameter $t_{X\text{-}Y}$ of Eq. (6) we employ the empirical sp^3s^* tight-binding model of Vogl *et al.*[29] Note that the universal model[29] provides only a simplified tight-binding theory of valence bands, as it cannot predict accurately the optical band gaps and underestimates the valence band offset for the GaAs/AlAs interface. However, as shown below, this model enables us to derive, in the most transparent way, the relation between the tight-binding matrix elements and coefficients in the boundary conditions for the envelope functions. For our purpose it is advantageous to consider instead of $|X\rangle$ and $|Y\rangle$ the basic states with the symmetry $\nu=\Delta_3,\Delta_4$, namely

$$|\Delta_3\rangle=\frac{1}{\sqrt{2}}(|X\rangle+|Y\rangle),|\Delta_4\rangle=\frac{1}{\sqrt{2}}(|X\rangle-|Y\rangle)$$

with a real or imaginary wave vector $\mathbf{k}\|[001]$. The hole wave function for a (001)-grown structure may be written as

$$\psi_\nu(\mathbf{r})=\sum_n C_n\phi_{n\nu}(\mathbf{r}-z_n\mathbf{e}_z) \tag{27}$$

with $z_n=na_0/4$ and $\mathbf{e}_z$ indicating the (001) direction. $\phi_{n\nu}$ are planar atomic orbitals at cation (n odd) or anion (n even) layers[30] and

$$C_n=\begin{cases}\eta_k(\varphi_k e^{ikz_n}+\varphi_{-k}e^{-ikz_n}) & \text{if } n \text{ is even,}\\ \xi_k\varphi_k e^{ikz_n}+\xi_{-k}\varphi_{-k}e^{-ikz_n} & \text{if } n \text{ is odd.}\end{cases} \tag{28}$$

The tight-binding Hamiltonian in the layer representation of $\phi_{n\nu}$ is obtained immediately from that of Ref. 29 by applying the unitary transformation from $|X\rangle$, $|Y\rangle$ to $|\Delta_3\rangle$, $|\Delta_4\rangle$ and considering different cations on either side of the interface at $n=0$. The corresponding set of coupled equations for C_n can be solved to express η_k and ξ_k in terms of tight-binding parameters:

$$\eta_k=\left(\frac{D_k+\Delta}{2D_k}\right)^{1/2},\quad \xi_k=-\eta_k\frac{V_k}{D_k+\Delta},$$

$$\Delta=\frac{1}{2}(E_c-E_a),\quad D_k=\sqrt{\Delta^2+|V_k|^2}, \tag{29}$$

$$V_k=U_-e^{ika_0/4}+U_+e^{-ika_0/4},\quad U_\pm=\frac{1}{2}(V_{xx}\pm V_{xy}).$$

E_c and E_a are the diagonal cation and anion energies, $V_{\alpha\beta}$ is the tight-binding-model matrix element between the anion p_α orbital and cation p_β orbital, in the notations of Ref. 29 $V_{xx}\equiv V(x,x),V_{xy}\equiv V(x,y)$. In the ''universal'' model[29] the empirical parameters are as follows: in GaAs $\Delta=1.314$ eV, $V_{xx}=1.955$ eV, $V_{xy}=5.078$ eV, and the corresponding set of parameters for AlAs is $\Delta'=1.302$ eV, $V'_{xx}=1.878$ eV, $V'_{xy}=4.292$ eV. Thus, the function $\psi_\nu(\mathbf{r})$ in Eq. (27) is a superposition of two normalized Bloch functions with the wave vectors $(0,0,k)$, $(0,0,-k)$ and the arbitrary superposition factors φ_k,φ_{-k}. The envelope wave function used in the effective mass approximation is given by (see, e.g., Ref. 31)

$$\varphi(z)=\varphi_k e^{ikz}+\varphi_{-k}e^{-ikz}. \tag{30}$$

Let us consider now an ideal pseudomorphic interface between GaAs and AlAs at $n=0$. The first boundary condition is the identity of the coefficients C_n at $n=0$ for the GaAs and AlAs materials. Following Ref. 1 we can write the second boundary condition as

$$U_- C_{-1} + (E_a^* - E) C_0 + U'_+ C_1 = 0 \quad \text{for } \Delta_3 \text{ solutions},$$

$$U_+ C_{-1} + (E_a^* - E) C_0 + U'_- C_1 = 0 \quad \text{for } \Delta_4 \text{ solutions}, \tag{31}$$

where $E_a^* = (E_a + E'_a)/2$ and the values for AlAs are labeled by a prime. Using Eqs. (28)–(31) and the energy dispersion of the Δ_3, Δ_4 valence states

$$E(k) = \frac{1}{2}(E_a + E_c) - D_k \tag{32}$$

one can transform Eq. (31) to an equation containing $\varphi(0) = \varphi_k + \varphi_{-k}$ and the first derivative $d\varphi(0)/dz = ik(\varphi_k - \varphi_{-k})$ at both sides of the interface:[32]

$$\eta \varphi_A = \eta' \varphi_B, \frac{1}{\eta}(\hat{v}_z \varphi)_A = \frac{1}{\eta'}(\hat{v}_z \varphi)_B \mp i \frac{\hbar t_{\mathrm{TB}}}{m_0 a_0} \eta' \varphi_B, \tag{33}$$

where the velocity operator $\hat{v}_z = -i(\hbar/M)\partial/\partial z$ with the energy-dependent velocity effective mass

$$\frac{1}{M(k)} = -\frac{V_{xx}^2 - V_{xy}^2}{D_k} \frac{a_0}{8\hbar^2 k} \sin\frac{k a_0}{2},$$

and

$$t_{\mathrm{TB}} = \frac{a_0^2 m_0}{2\hbar^2}\left(\frac{V_{xx} V_{xy}}{D_k + \Delta} - \frac{V'_{xx} V'_{xy}}{D'_k + \Delta'}\right). \tag{34}$$

In the basis $|X\uparrow\rangle$, $|Y\uparrow\rangle$ or $|X\downarrow\rangle$, $|Y\downarrow\rangle$, the boundary conditions for the two-component envelope $\mathbf{F} = (F_X, F_Y)$ take the form

$$\eta \mathbf{F}_A = \eta' \mathbf{F}_B, \frac{1}{\eta}(\hat{v}_z \mathbf{F})_A = \frac{1}{\eta'}(\hat{v}_z \mathbf{F})_B + i \frac{\hbar t_{\mathrm{TB}}}{m_0 a_0}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}(\eta' \mathbf{F}_B). \tag{35}$$

In the model under consideration the parameter $V_{xx}/(D_k + \Delta)$ and the factor η_k at $k \approx 0$ in both materials are close to each other and the boundary conditions (35) can be approximated by Eqs. (2) and (6) with

$$t_{X\text{-}Y} \approx \eta_0^2 t_{\mathrm{TB}}. \tag{36}$$

As a result, for the AlAs/GaAs pair, we obtain an estimated value of $t_{X\text{-}Y} \approx 0.76$.

VII. CONCLUSION

The symmetry considerations show that hh- and lh-states are coupled on the (001) interfaces of zinc-blende-based heterostructures even for vanishing in-plane wave vector. This kind of hh-lh mixing was previously reported as a result of tight-binding and pseudopotential calculations.[15,16,21] We have extended the EFA approach in which the hh-lh mixing under normal incidence is described by introducing off-diagonal terms in boundary conditions for the envelope functions. The boundary conditions have been written in the bases corresponding both to the direct product of Γ_6 and Γ_5 representations and to its decomposition into Γ_8 and Γ_7 spinor representations. The additional terms in the boundary conditions are equivalent to including an off-diagonal δ-function contribution to the hole effective Hamiltonian. The generalized EFA reproduces rather well microscopic model calculations of interband optical matrix elements in GaAs/AlAs(001) superlattices[16] and hole reflection from a GaAs/AlAs(001) single heterointerface.[15] From comparison with experiment and other theoretical models we have estimated the heavy-light hole mixing coefficient as $t_{l\text{-}h} = 0.5$ (the best fit with experimental data on anisotropic exchange splitting of excitonic levels in type II GaAs/AlAs superlattices), 0.9 (fitting the off-diagonal reflection spectra[15]), 0.32 (the best agreement with Ref. 16). Finally, a simple tight-binding model has been used to establish a direct relation between the mixing coefficient $t_{X\text{-}Y}$ and tight-binding matrix elements. The estimation of $t_{X\text{-}Y}$ by using Eq. (36) gives a value of 0.76 or $t_{l\text{-}h} = 0.44$ in reasonable agreement with the above values.

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