$\|\neq 0$), however, the wave functions e_{InAs} and h_{GaSb} have the same symmetry, so they anticross. This opens up a "hybridization gap" at some $\mathbf{k}_{\|} = \mathbf{k}_{\|}^*$. Using a pseudopotential plane-wave approach as well as a (pseudopotential fit) eight-band $\mathbf{k} \cdot \mathbf{p}$ approach, we predict the hybridization gap and its properties such as wave-function localization and out-of-plane dispersion. We find that recent model calculations underestimate this gap severely.

I. INTRODUCTION

On an absolute energy scale, the valence-band maximum (VBM) of GaSb is higher in energy than the conductionband minimum (CBM) of InAs.¹ Consequently, a GaSb/InAs heterojunction should be metallic, with the InAs-localized electron levels e_{InAs} below the GaSb-localized hole level h_{GaSb} . In (InAs)_n/(GaSb)_n superlattice geometry, quantum confinement will push e_{InAs} to higher energies and h_{GaSb} to lower energies, thus opening up a semiconducting band gap at sufficiently small periods $n < n_c$. Early experiments^{2,3} indeed suggested a transition from semiconductor at $n < n_c$ to semimetal at $n > n_c$. However, in 1983, Altarelli⁴ pointed out that even for $n > n_c$ there could be a semiconducting gap: since at some in-plane wave vector \mathbf{k}_{\parallel} the states e_{InAs} and h_{GaSb} have the same symmetry representation, they must an*ticross* (rather than cross), thus opening a finite gap. [Here $\mathbf{k}_{\parallel} = (k_x, k_y)$ indicates the transverse, two-dimensional wave vector parallel to the substrate plane, while k_z denotes the wave vector component parallel to the superlattice growth direction. The Brillouin zone is shown in Fig. 1.] Performing calculations in the $\mathbf{k} \cdot \mathbf{p}$ envelope function approximation (EFA), Altarelli⁴ found indeed a semiconducting gap even for $n > n_c$ at some in-plane wave vectors \mathbf{k}_{\parallel}^* . Previous experimental observations of semimetallic behavior^{2,3} were interpreted by Altarelli⁴ as being due to the abundant defects that fill in the band-gap region. In 1997, Yang et al.⁵ indeed detected, using capacitance-voltage measurements on $(InAs)_{46}/(GaSb)_{14}$ superlattices, a small band gap $(\approx 4 \text{ meV})$ in the in-plane dispersion. This has prompted theoretical interest in predicting the semiconducting gap of nominally semimetallic superlattices.⁶⁻⁸ In this paper we use a pseudopotential plane-wave approach to predict the hybridization gap and its properties such as wave function localization and dispersion relations. We also compare our results to those obtained by approximate models such as eight-band $\mathbf{k} \cdot \mathbf{p}$ (finding good agreement, provided that the parameters are drawn from pseudopotential calculations), and to a recent model calculation by de-Leon et al.⁶ (finding poor agreement). We also find that whereas Altarelli's model predicts but one hybridization gap thus suggesting semiconducting (rather than semimetallic) behavior at $n > n_c$, our multiband model shows that for long period superlattices there are multiple anticrossings. This would lead to a quasisemimetallic behavior, not semiconducting.

II. SYMMETRY-MANDATED BAND COUPLING AND ANTICROSSING IN III-V SUPERLATTICES

Since the semiconducting gap represents anticrossing between two levels, one must understand and predict the effective coupling potential $V_{e-hh}^{(n)}(\mathbf{k}_{\parallel},k_z)$ between the relevant anticrossing states.

There are three outstanding problems of anticrossing and band coupling in semiconductor superlattice physics, that were treated in the past by the "standard model," i.e., EFA.

(i) The $\Gamma - X$ coupling $V_{\Gamma,X}$ in $(AlAs)_n/(GaAs)_n$ (001) superlattices, which leads to anticrossing of Γ_{1c} -like and



FIG. 1. Brillouin zone for the tetragonal symmetry of the $(InAs)_n/(GaSb)_m$ (001) superlattices. The crystal primitive cell along the *z* axis is of length $L_z = (n+m)a$ and *a* is the zinc-blende lattice constant.

X



FIG. 3. Evolution of the wave function of the last occupied state (left column) and the first unoccupied state (right column) of the (InAs)₄₆(GaSb)₁₄ (001) superlattice along the in-plane $\mathbf{k}_{\parallel} = (k_x = k_y)$ direction at $k_z = 0$. Wave functions are averaged over the in-plane coordinates.

thicknesses n and m are changed. We have considered a $(InAs)_{30}/(GaSb)_{30}$ superlattice with the same total n+m period as the previously studied (InAs)₄₆/(GaSb)₁₄ superlattice. The pseudopotential calculated in-plane dispersion relations of the two superlattices along the $k_x = k_y$ direction at $k_z = 0$ are compared in Fig. 4. Since the well widths determine the confinement energies, using the (30,30) period rather than (46.14) leads to a more confined electron (since the InAs electron well is now narrower) and to a less confined heavy hole (since the GaSb hole well is now wider). Thus, the (30,30) superlattice has a smaller (negative) gap at $\mathbf{k}_{\parallel} = 0$ than the (46,14) superlattice. The negative gap at \mathbf{k}_{\parallel} =0 is now 17 meV, i.e., about one-fourth of the corresponding gap of the (46,14) superlattice. Since the electron and heavy-hole bands are already closer to each other at $\mathbf{k}_{\parallel} = 0$ than in the (46,14) case, the anticrossing point \mathbf{k}_{\parallel}^* occurs

TABLE I. Pseudopotential (*P*) and $\mathbf{k} \cdot \mathbf{p}$ calculated hybridization (*H*) gaps for a (InAs)₄₆(GaSb)₁₄ (001) superlattice. The band offset between the strained InAs CBM and GaSb VBM is 190 meV. In parentheses we give the band gaps obtained with a 150-meV offset.

Method	$E(\mathbf{k}_{\parallel}=0) \text{ (meV)}$		$E_H(\mathbf{k}_{\parallel} = \mathbf{k}^*) \text{ (meV)}$	
	$k_z = 0$	$k_z = \frac{\pi}{L_z}$	$k_z = 0$	$k_z = \frac{\pi}{L_z}$
P theory $\mathbf{k} \cdot \mathbf{p}$	65 68(32)	45 38(8)	25 29(22)	8 8(1.5)



FIG. 4. Comparison between the pseudopotential calculated dispersion relations of a $(InAs)_{46}(GaSb)_{14}$ superlattice and of a $(InAs)_{30}(GaSb)_{30}$ along the $(k_x = k_y)$ direction at $k_z = 0$.

closer to the Brillouin zone center. However, we see that the interaction V_{e-hh} in this region given by the pseudopotential theory is relatively strong, and, as a consequence, the hybridization gap is 15 meV wide, not much smaller than the negative gap at $\mathbf{k}_{\parallel} = 0$.

We have also examined the interband transition dipole matrix elements for the (30,30) superlattice and found that, while the transitions at $\mathbf{k}_{\parallel}=0$ have the same intensity as those in the (46,14) superlattice, both the intensity and the polarization anisotropy of the transitions at \mathbf{k}_{\parallel}^* are smaller that those we have found in the (46,14) superlattice. Thus, we see that, the closer E_H is to $\mathbf{k}_{\parallel}=0$, the less intense and anisotropic are the interband transitions.

E. Comparison of pseudopotential and model calculations

Figure 5 compares the pseudopotential results with the model calculation of de-Leon et al.⁶ for the (InAs)₄₆(GaSb)₁₄ system. The model of Ref. 6 describes the system as an InAs electron well interacting with a GaSb hole well, both wells being sandwiched between infinite barriers. Although two coupled quantum wells are a very simplified model of the system we are studying here, it is instructive to compare qualitatively our calculation with this model. The two systems are different in that the (InAs)₄₆(GaSb)₁₄ superlattice is a periodic system, showing a dispersion of the electron and hole bands along the k_z direction while there is no k_z dependence in the model of Ref. 6. The existence of the dispersion along k_z in our calculation reveals a coupling with other bands. In Ref. 6 the only allowed coupling is limited to the two electron and hole ground states of the uncoupled wells.

In Fig. 5 we compare the in-plane dispersions of the model in Ref. 6 with the superlattice dispersion for $k_z=0$. We see that the values of \mathbf{k}_{\parallel}^* at the anticrossing points are similar in both calculations. We can think of our $k_z=0$ superlattice wave function as a periodic repetition of the corresponding quantum well wave function without any complication of additional phase factors. Now, however, in addition to the mixing due to the perturbation at the InAs/GaSb interface, which is present in the model of Ref. 6, we have an additional perturbation at the GaSb/InAs interface. As a re-

sult, the anticrossing gap at ${\bf k}$