2_V symmetry of a superlattice with no-common-

atom such as InAs/GaSb from the D_{2d} symmetry of a superlattice that has a common atom, e.g., InAs/GaAs. Consequently, **k**•**p** lacks the strong in-plane polarization anisotropy of the interband transition evident in the pseudopotential calculation. Since the pseudopotential band gap is larger than the **k**•**p** values, and most experimental band gaps are even smaller than the **k**•**p** band gap, we conclude that to understand the experimental results one must consider physical mechanisms beyond what is included here (e.g., interdiffusing, rough interfaces, and internal electric fields), rather than readjust the $\mathbf{k} \cdot \mathbf{p}$ parameters. $\left[S0163 \text{--} 1829(99)07531 \text{--} 1 \right]$

I. INTRODUCTION

 $(InAs)_n / (GaSb)_m$ forms an interesting superlattice and quantum-well system, because for large periods $(n,m) \rightarrow \infty$ this heterojunction has a *negative* band gap (the InAs conduction band minimum is \sim 160 meV below the GaSb valence band maximum), while for smaller periods, quantum confinement of InAs electrons and GaSb holes leads to finite, positive band gaps $E_g(n,m)$ of up to \sim +400 meV. Thus, by selecting (n,m) , one can construct lasers and detectors at technologically useful, tunable IR wavelengths.^{1,2} The design of such structures relies on the accurate modeling of $E_g(n,m)$. This has been largely done in the past via the $\mathbf{k} \cdot \mathbf{p}$ effective mass approximation.^{3–5} at the Brillouin zone center

more than 8 bulk bands at are needed to reduce the error to \sim 10–20 meV. The basic reason for this that just a few zinc-blende Bloch states drawn from lihpoint are not enough to describe the dff $(i.e, k > k_c)$ states. Thus, 16 0 TD 1 -1.16 momentum bulk Bloch state

^c . However, technologically useful IR wavelengths in (InAs)*ⁿ* /(GaSb)*^m* typically require rather small periods (*n*,*m*) of 4–12 ML.

(ii) In the $\mathbf{k} \cdot \mathbf{p}$ method the Γ Bloch functions of the constituents are implicitly assumed to be equal, e.g., u_{Γ} (GaAs) $= u_{\Gamma}(InAs)$. This neglects the chemical uniqueness of the wave functions of the heterojunction partners. This approximation u_{Γ} (AB) = u_{Γ} (CD) then implies that a carrier traveling from material AB to CD sees, in the **k**•**p** method, a potential barrier that equals the AB/CD band offset, while in reality, if u_{Γ} (AB) $\neq u_{\Gamma}$ (CD) there is an additional effective potential barrier, as discussed by Burt.⁹

(iii) The $\mathbf{k} \cdot \mathbf{p}$ fails to recognize atomistic details. It thus treats a C_{2v} -symmetric no-common-atom superlattice¹⁰ such as $(InAs)_n / (GaSb)_m$ as if it was a D_{2d} -symmetric, commonatom superlattice such as $(InAs)_n / (GaAs)_m$ $(InSb)_n$ /(GaSb)_{*m*}. In a common-atom superlattice such as $(Insb)_n / (GaSb)_m$, the two interfaces are symmetry equivalent, i.e., the one with $[110]$ In-Sb bonds plus $[\overline{1}10]$ Ga-Sb bonds is equivalent to the other one with $\overline{[10]}$ In-Sb bonds plus $[110]$ Ga-Sb bonds. As a result, in this D_{2d} -symmetry

 $_0=0$, the wave vector distance $\mathbf{k}_c - \mathbf{k}_0$, outside which significant errors in the bulk eight point group operations), the two in-plane directions

dispersion relationship can be seen, is sometimes surprisingly small(see Ref. 6 for GaAs and AlAs, Ref. 7 for InP and CdS ϕ . An extreme case is the zinc-blende state, where the eight-band**k**•**p** method overestimates its position by6 9 eV in GaSb, 5 eV in InAs and 25 eV in GaAs. Many

face has $\overline{[110]}$ Ga-As bonds and $\overline{[110]}$ In-As bonds. As a result, the two in-plane directions $\begin{bmatrix} 110 \end{bmatrix}$ and $\begin{bmatrix} \overline{1}10 \end{bmatrix}$ are inequivalent,^{11–14} and the symmetry is reduced to C_{2v} (four point group operations). Similarly, the $\mathbf{k} \cdot \mathbf{p}$ does not recognize the proper odd-even symmetry of a film made of an odd or even number of monolayers,¹⁵ or the correct C_{2v} symmetry of a self-assembled InAs/GaAs pyramidal dot.¹⁶ The existence of a lower, C_{2v} symmetry in InAs/GaSb superlattices than the one (D_{2d}) assumed in standard $\mathbf{k} \cdot \mathbf{p}$ method has $several$ consequences. (a)

~b! In our methodology the **k**•**p** parameters are viewed as fixed constants not as adjustable parameters. Once determined from the bulk band structures (drawn from wellestablished experiments and state-of-the-art *ab initio* calculations, see below) they have not been readjusted to fit the superlattice experimental data, or the superlattice pseudopotential calculation. Indeed, in **k**•**p** theory the input parameters are fundamentally bulk quantities, not properties of the nanostructures themselves.

II. METHOD OF CALCULATION

We first determine screened pseudopotentials $\{v_\alpha(q)\}$ as a function of momentum *q* for α = Ga, In, As, Sb, using them to calculate the bulk band structures of GaSb and InAs from which we find the **k**–**p** band parameters shown in Table I. These parameters are then used in an eight-band $\mathbf{k} \cdot \mathbf{p}$ model⁴ to calculate the superlattice states. Separately, the pseudopotentials $\{v\}$

all-electron calculation the anion *p*-cation *d* coupling is fully

above (below) the InAs CBM (GaSb VBM) constitutes the electron (hole) confinement energy. We see that the pseudo-

This analysis suggests that new physical effects, thus far neglected, might need to be considered. For example, current pseudopotential and $\mathbf{k} \cdot \mathbf{p}$ calculations assume abrupt interfaces, while experiment $19,37,38$ points to inter-diffused and rough interfaces^{19,37} island formation³⁸⁻⁴⁰ and even compositional modulation, 38 which have been shown in other shortperiod superlattice systems to lead to large band gap reductions. Another possibility is the internal electric field allowed by the C_{2v} symmetry of the system. To estimate the effect of internal electric field on the band gap reduction we have compared the LDA calculated band gap of $(InAs)_7InSb(GaSb)_8$ and $GaAs(InAs)_8(GaSb)_7$ with that of $(InAs)_{8}(GaSb)_{8}$. The former two structures have equivalent interfaces, and thus no electric field is induced by the interface. We find that the internal electric field reduced the band

gap by about \sim 20 meV, thus, it does not appear to be a dominant effect that would explain the large discrepancy between present calculations and experimental observations.

To date, there is not enough data on intervalence energy splittings available to allow a meaningful comparison with experiment. Such experiments are called for, so that comparison with the values published here can be made.

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