face has $[\overline{1}10]$ Ga-As bonds and $[110]$ In-As bonds. As a result, the two in-plane directions $[110]$ and $[\overline{1}10]$ 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 $\mathbf{k}\cdot\mathbf{p}$ parameters are viewed as fixed constants not as adjustable parameters. Once determined from the bulk band structures (drawn from well-established 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 $\mathbf{k}\cdot\mathbf{p}$ 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 $\alpha =$ Ga, In, As, Sb, using them to calculate the bulk band structures of GaSb and InAs from which we find the $\mathbf{k}\cdot\mathbf{p}$ band parameters shown in Table I. These parameters are then used in an eight-band $\mathbf{k}\cdot\mathbf{p}$ model[4] 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-

that there is a finite amplitude there (unlike hh2 at $n=20$). Such zone center lh-hh mixing and anticrossing are absent in the $\mathbf{k}\cdot\mathbf{p}$ calculation. It is interesting to note, however, that this anticrossing does exist in $\mathbf{k}\cdot\mathbf{p}$ at off Γ in-plane wave vectors. The quantitative difference in the lh energy levels (Table III) between pseudopotential and $\mathbf{k}\cdot\mathbf{p}$ ranges from 145 meV at $n=1$ to 9 meV at $n=20$.

IV. SUMMARY

The following points emerge from the comparison of pseudopotential and $\mathbf{k}\cdot\mathbf{p}$ results.

(1) The $\mathbf{k}\cdot\mathbf{p}$ underestimates the electc39kabatesof61 T84J -1.2 -1.16652.8(en394-412.394-345.2(94-super(ca5.54(there)]TJ /F58 06f 1.6
$k\cdot\mathbf{p}$