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-

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 formation[38–40] and even compositional modulation,[38] which have been shown in other short-period 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.

ACKNOWLEDGMENTS

The work at NREL was supported by the U.S. Depart-