

## New method for calculating electronic properties of superlattices using complex band structures

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The electronic structure of semiconductor superlattices is analyzed in terms of complex bulk band structures. The details of the complex bands and the matching conditions at the interfaces are found to be crucial in energy ranges of experimental interest. The limits of applicability of the Kronig-Penney and two-band models are shown.

A wide variety of phenomena in semiconductor superlattices has been investigated experimentally in recent years.<sup>1,2</sup> As long as the widths of the alternating superlattice layers were large ( $\geq 100$  Å), analysis of the conduction- and valence-band-edge electronic structure in terms of the Kronig-Penney (KP) or two-band models was adequate.<sup>1-5</sup> More detailed calculations for thinner layers using empirical tight-binding<sup>6</sup> or pseudopotential methods<sup>7</sup> were possible, but lacked the intuitive clarity of the simpler models. Without a clear physical basis for the choice of the parameters in the tight-binding or pseudopotential models, wide disagreement over such basic properties as band gaps was possible.<sup>8</sup>

In this paper we introduce a new method for solving the superlattice tight-binding Hamiltonian. It incorporates the detailed descriptive ability of previous tight-binding methods with the intuitive clarity of the simple KP and two-band models. For the first time, superlattices with arbitrary layer thicknesses are represented by full (at least  $s$ ,  $p_x$ ,  $p_y$ , and  $p_z$  orbitals per atom) tight-binding Hamiltonian matrices of the same dimension (30  $\times$  30 in this case). Unlike methods employing Green's functions, the electronic states are found directly.

Using this method, the limits of applicability of the simpler models can be investigated and understood in terms of complex bulk band structures. We present here the results of a calculation

for the GaAs-AlAs(100) superlattice and compare them with the results of the simpler models. The concepts involved can be applied to other semiconductor superlattices as well.

An empirical tight-binding Hamiltonian with nearest-neighbor interactions and including excited anion and cation  $s$  states in addition to the normal  $s$ ,  $p_x$ ,  $p_y$ ,  $p_z$  basis is used.<sup>9</sup> The excited  $s$  states allow the lowest bulk conduction band to be fit well. For the superlattice, the on-site parameters of the interfacial As atoms are taken to be the average of those in bulk GaAs and AlAs.

To find the superlattice states and energies, an initial estimate of the energy,  $E$ , of the superlattice state of interest is chosen. Next, the bulk states in both constituent materials, including evanescent waves, with that energy are found. This is accomplished by solving the bulk tight-binding Schrödinger equation,  $\det[H(\vec{k}_\parallel, k_z) - E] = 0$ , for both GaAs and AlAs. Here,  $\vec{k}_\parallel$  and  $k_z$  are bulk  $k$  vectors parallel and perpendicular to the interface.  $E$  and  $\vec{k}_\parallel$  are specified and  $k_z$  is found by solving the polynomial equation resulting from the determinant or from an equivalent eigenvalue equation.<sup>10</sup>

The superlattice state is then expanded in terms of the ten GaAs and ten AlAs bulk states ( $\psi_n^{(\sigma)}$ ;  $\sigma = 1, 2$ ;  $n = 1-10$ ), and ten As orbitals summed over atomic sites in the interface plane ( $\phi_\alpha^{(\sigma)}$ ;  $\sigma = 1, 2$ ;  $\alpha = 1-5$ ) (five at each inequivalent interface):

$$\Psi_q(\vec{r}) = \sum_L e^{iqL} \sum_{\sigma=1}^2 \left( \sum_{n=1}^{10} C_n^{(\sigma)} \psi_n^{(\sigma)}(\vec{r} - L\hat{z}) + \sum_{\alpha=1}^5 d_\alpha^{(\sigma)} \phi_\alpha^{(\sigma)}[\vec{r} - (L + t^{(\sigma)}\hat{z})] \right).$$

Here  $\hat{z}$  is the direction perpendicular to the interfaces,  $q$  is the superlattice wave vector in the  $\hat{z}$  direction,  $L$  denotes the superlattice unit-cell position,  $C_n^{(\sigma)}$  and  $d_\alpha^{(\sigma)}$  are the expansion coefficients of the bulk states and As planar orbitals, and  $t^{(\sigma)}$  denotes the position of each of the two interfaces in a unit cell.

The coefficients are determined by diagonalizing the superlattice Hamiltonian using this basis set.<sup>11</sup>

Since, in general the resulting superlattice state energy,  $E_s$ , is not the same as  $E$ , this procedure must be iterated until the two energies coincide.

The advantage of this method is that since the superlattice state is found as a linear combination of bulk states with complex  $\vec{k}$ , the complex bulk band structures provide a simple physical guide in understanding the electronic structure. Figure 1 shows the complex band structures of GaAs

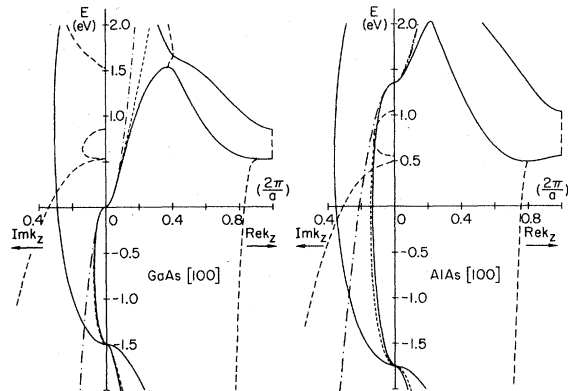


FIG. 1. Complex band structures of GaAs and AlAs along the [100] direction. Both the real bands ( $\text{Im} k_z = 0$ ) and the purely imaginary bands ( $\text{Re} k_z = 0$ ) are denoted by solid lines. The complex bands ( $\text{Re} k_z \neq 0$  and  $\text{Im} k_z \neq 0$ ) are denoted by pairs of long dashed lines. The lines associated with  $\text{Re} k_z$  and  $\text{Im} k_z$  are plotted in the right and left portion of each figure, respectively. Also included are the corresponding band structures for Kronig-Penney (dash-dotted) and two-band (short dash) models. Energy is relative to the GaAs conduction-band minimum.

and AlAs in the [100] direction in the energy range of their band gaps. Energy bands with nonzero values for the imaginary part of  $\vec{k}$  are seen to emanate from the extrema of the conventional real bands.<sup>12</sup> The complex band structures in the energy range of the conduction-band minima are of particular interest in analyzing the low-lying superlattice conduction states. There are two important bands in this region: one which connects the direct valence-band maximum and conduction-band minimum and one which connects with the X-point conduction-band minimum. The third band shown does not contribute to the superlattice conduction-band-minimum state by symmetry. The superlattice valence-band maximum states can similarly be analyzed by examining the complex bulk valence-band structure. However, since the spin-orbit interaction (omitted in this calculation) is important in determining the valence-band-edge structure, these states are not adequately described in this model.

The limitations of the KP and two-band models can now be discussed. The first difficulty is that the Kronig-Penney model does not describe the  $E$  vs  $\vec{k}$  relationship in the bulk material correctly for complex  $k_z$ . For example, Fig. 1 compares the KP parabolic dispersion curves with the tight-binding results. For energies near the GaAs conduction-band edge (the bottom of the "well") the KP model predicts too large a value for imaginary  $k_z$  in AlAs. Therefore, the decay lengths of the superlattice states in the AlAs layers will

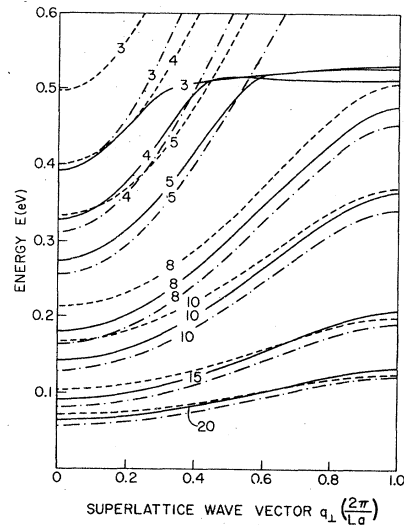


FIG. 2. Superlattice conduction-band-minimum dispersion curves in the  $\hat{z}$  direction for superlattices with two layers of AlAs alternating with  $N$  layers of GaAs.  $N = 3, 4, 5, 8, 10, 15, 20$  as indicated. Solid curve: tight binding. Dashed curve: Kronig-Penney. Dash-dotted curve: two-band model. Energy is relative to the GaAs conduction-band minimum.  $L$  is the total number of alternating GaAs and AlAs layers.

be too short. This should lead to superlattice energies which are too high. The KP interfacial boundary conditions (matching the wave function and its derivative) are also in serious error. More detailed studies<sup>13</sup> demonstrate that the KP boundary conditions are the limits of one-band tight-binding boundary conditions with unrealistically large transfer matrix elements. This tends to lower the superlattice energies somewhat.<sup>13</sup>

The two-band model is a better approximation in that it can describe correctly the complex band which connects the bulk conduction and valence bands at the zone center. Furthermore, it does not have KP boundary conditions. With properly chosen parameters, the decay lengths for that band in the AlAs layers can, therefore, be accurately described. The GaAs dispersion curve will also be improved over the KP result. The two-band dispersion curve within the band gaps is shown in Fig. 1.<sup>14</sup> The two-band-model parameters were chosen to produce the average of the conduction and light-hole effective masses and the correct band gaps and band discontinuities.

Figure 2 compares the results of calculations obtained using the tight-binding, KP, and two-band models. Shown are the superlattice conduction-band-minimum dispersion curves in the  $z$  direction for superlattices consisting of two layers of AlAs alternating with a varying number of GaAs layers. For a large number of GaAs layers, all

three models give similar results. As the number of GaAs layers is decreased, the KP model energies increase faster than those predicted by the two-band and tight-binding models. In addition, while the discrepancy between the tight-binding and two-band-model results are approximately constant across the band, the KP energies have somewhat less dispersion. At energies approaching and above the bulk  $X$ -point conduction-band-minimum energy ( $\sim 0.52$  eV in both GaAs and AlAs), both the KP and two-band-model curves diverge from the tight-binding curve. Below this energy, the two-band model is a reasonable approximation to the more complete tight-binding model.

The failure of the two-band model near that energy is due to its inability to describe the complex bands emanating from the  $X$ -point conduction-band minima. At these energies the superlattice state has a large component of bulk states with complex  $\vec{k}$  near the  $X$  point and therefore it cannot be ignored. Since the  $X$ -point energy is much less than the AlAs direct gap energy, this occurs much below the top of the direct conduction-band well. The tight-binding superlattice dispersion curve flattens out as soon as the  $X$ -point energy is reached.<sup>3</sup>

Finally, we compare the results of our calculation with available data. Table I shows the theoretical and experimental band-gap energies of several GaAs-AlAs superlattices. Overall agreement is good. Discrepancies are most likely due to the experimental uncertainties in the determination of band gaps and layer thicknesses and in the inherent approximations of the tight-binding method.

In summary, we have developed a new technique for calculating superlattice electronic structure

TABLE I. Theoretical and experimental values of the band gaps of GaAs-AlAs superlattices with  $M$  layers of GaAs alternating with  $N$  layers of AlAs.

Theory		Experiment	
$M/N$	$E_{\text{gap}}$	$M/N$	$E_{\text{gap}}$
6/3	1.87	6.13/3.37	1.85 <sup>a</sup>
7/4	1.87	7.3/4.4	1.90 <sup>b</sup>
9/4	1.79	9.4/3.85	1.77 <sup>b</sup>
18/4	1.63	17.67/3.53	1.66 <sup>c</sup>
19/9	1.64	18.73/8.83	1.65 <sup>c</sup>
16/16	1.68	15.9/15.9	1.63 <sup>d</sup>
11/18	1.78	10.60/17.67	1.81 <sup>c</sup>

<sup>a</sup>Reference 15.

<sup>b</sup>Reference 16.

<sup>c</sup>Reference 17.

<sup>d</sup>Reference 18.

within the tight-binding approximation. It has been used to explore the limitations of simpler models in terms of complex bulk band structures. The KP model fails to describe the superlattice state in the AlAs layers and uses incorrect boundary conditions. The two-band model can provide an approximate description of the complex band structure for superlattice energies near the GaAs conduction-band minimum. For superlattice energies near and above the bulk  $X$ -point energies, and elsewhere, the more complete tight-binding model is necessary.

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order to reproduce experimental values of the effective masses in GaAs and AlAs, band gaps, and band discontinuities.

<sup>10</sup>This was first accomplished for a full tight-binding Hamiltonian by G. C. Osbourn and D. L. Smith, Phys. Rev. B **19**, 2124 (1979). A more efficient method for solving the determinantal equation and a method which finds  $e^{i\vec{k}\cdot\vec{a}/2}$  ( $a$  being the lattice constant) directly from an eigenvalue equation will be presented in future papers.

<sup>11</sup>Orthonormal linear combinations of the  $\psi_n^{(\sigma)}$  are used.

<sup>12</sup>This and other details will be discussed in a subsequent paper.

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