Brillouin-zone Unfolding of Perfect Supercells Having Nonequivalent Primitive Cells Illustrated with a Si/Ge Tight-Binding parameterization

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I. INTRODUCTION

Most semiconductor nanostructures are made from materials which adopt a rectangular geometry of some sort. For example, fcc is the lattice for the most common semiconductors: Si (diamond) and GaAs (zinc blende). In addition, many technologically important nanostructures such as superlattices (SLs), resonant-tunneling diodes, ultrascalled metal-oxide-semiconductor field-effect transistors, quantum wells, and nanowires are constructed as layers, so that the rectangular geometry persists, even in the presence of strain. Embedded objects such as self-assembled quantum dots are also easily modeled with rectangular unit cells of differing composition. Due to the rectangular geometry, grouping atoms into eight-atom zinc-blende-like conventional unit cells yields a simplified treatment and storage scheme for relative atom coordination. The result is generally more efficient and easily debugged algorithms, making the choice attractive from a computational perspective as well. A rectangular cell—even a nonprimitive one—is therefore a natural choice for the underlying building block of a general nanodevice modeling tool such as NEMO3D.\textsuperscript{1,2}

Although using a nonprimitive rectangular unit cell to calculate $E(k)$ relations for superlattices or bulk semiconductors simplifies the boundary conditions, the results can be difficult to relate back to the primitive-cell $E(k)$ relations due to zone folding. The zone-unfolding process is more complicated if the true primitive cell is not rectangular. For bulk semiconductors such as Si or GaAs, the conventional fcc unit cube contains four identical primitive cells (rhombahedra), and the periodic boundary conditions are applied over the cube instead of over $N_i$ primitive cells along each of the (nonorthogonal) primitive cell vectors $a_i$. For this case, our zone-unfolding method\textsuperscript{3} can be used in its original formulation, but with a different choice of allowed wave vectors.\textsuperscript{4,5}

A more difficult complication arising from the use of a nonprimitive rectangular cell can occur in modeling superlattices. A specific example is the Si(4)Ge(4) SL fabricated and studied experimentally by Pearsall et al.\textsuperscript{6} and theoretically using the linear muffin-tin orbital (LMTO) method by Ikeda et al.\textsuperscript{7} Each primitive cell of this SL has eight atoms, so a natural choice for a nonprimitive rectangular cell is a stack of two eight-atom rectangular cells. Were strain absent, each eight-atom rectangular cell would simply be a conventional fcc cube. This rectangular cell is by far the easiest to implement, since its faces are perpendicular to the Cartesian axes. Moreover, it is compatible with many common nanodevice geometries.

Unfortunately, it is not compatible with this SL, since two identical SL primitive cells do not fit into this “conventional” nonprimitive cell as shown in Fig. 1. The filled atoms (striped for Si, dotted for Ge) belong to the two primitive SL unit cells (transparent rectangular boxes). Open atoms belong to other SL primitive cells and are shown to delineate the boundaries of the nonprimitive rectangular cell. The atoms of cell 0 (forward SL primitive cell) are labeled $j=0,\ldots,7$; the atoms of cell 1 (rearward SL primitive cell) are not labeled. Observe that atoms 3 and 7 of SL primitive cell 1 actually lie outside the rear face of the nonprimitive rectangular cell. Thus, two identical primitive cells of this SL do not fit into a conventional, rectangular nonprimitive cell.

If one allows the two SL primitive cells to differ, then both can be contained in the conventional rectangular cell, as shown in Fig. 2. This nonprimitive rectangular cell also contains 16 atoms, with indices as $(n,j)$, $n=0,1$, $j=0,\ldots,7$, where $n$ is the SL primitive-cell index and $j$ the index of the atom within the cell. Note that the two SL primitive cells of Fig. 2 are different. Cell 0 is identical to the forward primitive cell of Fig. 1 (cell with numbered atoms). Cell 1 has atoms 2, 3, 6, and 7 translated $a_\perp$ relative to their counter-
not equivalent, the method for zone unfolding is not immediately obvious.

The dilemma posed by the rectangular cell of Fig. 2 needs resolution, since it is impractical to change the primitive-cell definition in a general nanostructure modeling tool. For the case of the SL discussed above, one solution would be to use a nonprimitive (and nonconventional) rectangular cell with $x$ and $y$ axes rotated by $45°$. However, doing so in a calculation based on conventional rectangular cells would require major alterations to the critical supercell electronic structure algorithm. If one must make such changes for each SL geometry, then the tool is hardly general. Because any rectangular unit cell chosen might well be suitable for some SLs but not for others, a better resolution is to find a method by which the primitive-cell bands may be recovered even with a unit cell like that in Fig. 2, where the primitive cells are different. This solution preserves the generality of the tool, since the underlying rectangular cell need not be changed and the SL-specific algorithmic modifications come after the electronic structure calculation.

In this work, we modify our Brillouin-zone-unfolding method\textsuperscript{3–5} so that it can recover the primitive cell $E(k)$ relations from a nonprimitive rectangular cell such as that in Fig. 2. We illustrate the method for the Si(4)Ge(4) SL studied in Refs. 6 and 7 using the $sp^3d^5s^*$ empirical tight-binding model\textsuperscript{8} with our room-temperature bulk Si and Ge parameters.\textsuperscript{9} Because strain is present in the SL, we provide here a set of strain parameters for Si and Ge which incorporates diagonal parameter shifts due to nearest-neighbor interactions. We find good agreement with the results of Refs. 6 and 7.

II. METHOD

A. Allowed wave vectors

The first step in recovering the primitive cell $E(k)$ relations from those of the nonprimitive cell is the determination of the allowed primitive-cell wave vectors and their relationship to the nonprimitive-cell wave vectors. As shown in Fig. 2, the nonprimitive rectangular cell has direct lattice vectors

$$\mathbf{A}_1 = a_1 \mathbf{e}_x, \quad \mathbf{A}_2 = a_2 \mathbf{e}_y, \quad \mathbf{A}_3 = a_3 \mathbf{e}_z,$$

whereas the primitive cell of Fig. 1 has direct lattice vectors

$$\mathbf{a}_1 = \frac{a_1}{2} (\mathbf{e}_x + \mathbf{e}_y), \quad \mathbf{a}_2 = \frac{a_2}{2} (\mathbf{e}_x - \mathbf{e}_y), \quad \mathbf{a}_3 = a_3 \mathbf{e}_z.$$

Thus, the nonprimitive cell is exactly twice the volume of the primitive cell. The primitive-cell reciprocal lattice vectors are therefore

$$\mathbf{b}_1 = \frac{2\pi}{a_1} (\mathbf{e}_x + \mathbf{e}_y), \quad \mathbf{b}_2 = \frac{2\pi}{a_2} (\mathbf{e}_x - \mathbf{e}_y), \quad \mathbf{b}_3 = \frac{2\pi}{a_3} \mathbf{e}_z.$$  

The primitive-cell Brillouin zone is thus a rectangular parallelepiped, rotated so that its projection in the $x$-$y$ plane is a diamond (Fig. 3). The Brillouin zone of the nonprimitive rectangular cell is also a rectangular parallelepiped, with sides perpendicular to the Cartesian axes. Figure 3 shows the
projections of these zones in the plane, the diamond being that of the primitive cell and the smaller inscribed square being that of the nonprimitive rectangular cell. Both zones have the same \( z \)-length: \(-\pi/a_x \leq k_z \leq \pi/a_x\).

The allowed wave vectors are determined by enforcing periodic boundary conditions on the wave function over an integral number of nonprimitive cells in each of the directions \( A_i, i = 1, 2, 3 \):

\[
\psi(r + N_i A_i) = \psi(r), \quad i = 1, 2, 3. \tag{4}
\]

These boundary conditions yield the familiar set of allowed supercell wave vectors \( \mathbf{K}_n, n = (n_1, n_2, n_3) \):

\[
\mathbf{K}_n = 2\pi \left[ \frac{n_1}{N_1} \mathbf{a}_1 + \frac{n_2}{N_2} \mathbf{a}_2 + \frac{n_3}{N_3} \mathbf{a}_3 \right],
\]

\[
n_j = \begin{cases} 
\frac{N_j}{2}, & N_j \text{ even}, \\
\frac{N_j - 1}{2}, & N_j \text{ odd}.
\end{cases} \tag{5}
\]

For each of the \( N_1 \times N_2 \times N_3 \) supercell wave vectors \( \mathbf{K}_n \), there must be two primitive cell wave vectors since each nonprimitive cell contains two primitive cells. One primitive-cell wave vector is obviously just \( \mathbf{K}_n \), since the nonprimitive-cell Brillouin zone is entirely contained within the primitive-cell Brillouin zone (Fig. 3). The other primitive-cell wave vector is found by applying periodic boundary conditions over a single nonprimitive cell, i.e., \( N_1 = N_2 = N_3 = 1 \) in Eq. (4). For the single nonprimitive cell, the only supercell wave vector is therefore \( \mathbf{K}_n = \mathbf{0} \), which is likewise one of the two allowed primitive-cell wave vectors. The other is the supercell reciprocal lattice vector \( \mathbf{G} = (2\pi/a_i) \mathbf{e}_i \), lying at the vertex of the primitive-cell Brillouin zone (Fig. 3), which satisfies periodic boundary conditions over the nonprimitive cell. This conclusion follows from writing the wave function in Bloch form:

\[
\psi(r) = e^{ik \cdot r} u_k(r), \quad u_k(r + N_i A_i) = u_k(r), \quad i = 1, 2, 3. \tag{7}
\]

\[
\Rightarrow \psi_G(r + a_i \mathbf{e}_i) = e^{i(2\pi/a_i)(s + n_i)} u_G(r + a_i \mathbf{e}_i) = e^{i(2\pi/a_i) s} u_G(r) = \psi_G(r). \tag{8}
\]

Because \( \mathbf{G} = (2\pi/a_i) \mathbf{e}_i \) obviously satisfies periodic boundary conditions over any integral number of nonprimitive cells in each of the directions \( A_i \), it follows that the allowed primitive-cell wave vectors are thus

\[
\mathbf{k}_{n,j} = \mathbf{K}_n + \mathbf{G}_j, \quad j = 0, 1, \quad \mathbf{G}_0 = 0, \quad \mathbf{G}_1 = \frac{2\pi}{a_i} \mathbf{e}_i. \tag{9}
\]

Note that it may be necessary to shift the \( \mathbf{k}_{n,j} \) back into the primitive-cell first Brillouin zone, but this is easily accomplished (see Ref. 4). Also, observe that \( (2\pi/a_i) \mathbf{e}_i \) is not independent since it differs from \( \mathbf{G}_1 \) by a primitive-cell reciprocal lattice vector: \( (2\pi/a_i) \mathbf{e}_i = \mathbf{G}_1 - \mathbf{b}_2 \).

### B. Modified projection method

Extracting the primitive-cell \( E(k) \) relations from those of the nonprimitive cell involves relating the wave functions in the nonprimitive rectangular cell basis and the primitive-cell basis. Because the two primitive cells in the rectangular cell of Fig. 2 are not identical, we adopt a slightly different notation from that employed in Refs. 3 and 5. An atomlike orbital in the \( \sigma \) basis (\( \rho \) for primitive, \( s \) for supercell or nonprimitive) is written as \( | \alpha; \mathbf{X}_{m,l,j}^\sigma \rangle \), where \( \alpha \) is a composite index encompassing the orbital type (\( s, p_x, p_y, \text{ etc.} \)), spin, and species, and \( \mathbf{X}_{m,l,j}^\sigma \) gives the atom location. The integer trio \( \mathbf{m} = (m_1, m_2, m_3) \) indexes a 16-atom rectangular cell, \( l \) indexes one of its two eight-atom primitive cells, and \( j \) indexes one of the eight atoms.

In the primitive-cell basis, the locations are specified as

\[
\mathbf{X}_{m,l,j}^\rho = \mathbf{R}_m + \rho_l + \delta_j, \tag{10}
\]

\[
\mathbf{R}_m = \sum_{j=1}^{3} m_j \mathbf{A}_j, \quad \rho_0 = 0, \quad \rho_1 = -a_1, \tag{11}
\]

where the nonprimitive and primitive direct lattice vectors are given in Eqs. (1) and (2). The exact specification of the \( \delta_j \) is not critical for deriving the method. Recall from the introduction that atoms 3 and 7 of primitive cell 1 for a given 16-atom rectangular cell \( \mathbf{m} \) actually lie outside the rear wall of the cell. This poses no difficulty, though, since we only use the rectangular cell to locate the origin (atom 0, primitive cell 0) of a pair of two identical primitive cells.

In the nonprimitive or supercell basis, the atom locations (see Fig. 2) are specified as

\[
\mathbf{X}_{m,l,j}^\rho = \mathbf{R}_m + \rho_l + \delta_j^\rho, \tag{12}
\]

where \( \mathbf{R}_m \) and \( \rho_l \) are defined in Eq. (11) above and

\[
\delta_j^{\rho} = \delta_j + a_1 e_\perp \Delta_j^{\rho}, \quad \Delta_j^{\rho} = \begin{cases} 
0, & l = 0, l = 1, j = 0, 1, 4, 5 \\
1, & l = 1, j = 2, 3, 6, 7.
\end{cases} \tag{13}
\]

Comparison of Eq. (10) and Eqs. (12) and (13) reveals that

\[
\mathbf{X}_{m,l,j}^\rho = \mathbf{X}_{m,l,j}^{\rho}, \quad l = 0; \quad l = 1, \quad j = 0, 1, 4, 5. \tag{14}
\]
\( X_{m,i,j}^* = X_{m,i,j} + \alpha_i e_z = X_{i(m_1+1,m_2,m_3),l}^* \), \( l = 1, 2, 3, 6, 7 \).

(15)

Equation (15) shows that on projection of the supercell state onto the primitive-cell basis, atom 2, 3, 6, and 7 of primitive cell 1 will receive an extra phase factor \( \exp(iK_d) \).

Projecting the primitive-cell states out of the supercell states proceeds as in Refs. 3 and 5 but subject to the modifications of Eqs. (10)–(15) above. The treatment here is specific to the nonprimitive rectangular cell of Fig. 2. For a SL composed of \( N_S \) nonprimitive rectangular cells, the supercell state of energy \( E_p \) is written as

\[
|\Psi_p(K)\rangle = \sum_{m} \sum_{\alpha} \sum_{l=0}^{7} \frac{1}{\sqrt{N_S}} \rho_{l,p}^{(\alpha)}(K) |\alpha;X_{m,l,j}^{e}\rangle,
\]

(16)

where there are \( N_{O,atom} \) orbitals per atom and the notation \( \langle \alpha | \) on the sum over \( m \) denotes the \( N_S \) trios \( m \) which index all rectangular cells of the SL. Cyclic boundary conditions are applied over the \( N_S \) rectangular cells.

The supercell states are projected onto the Bloch basis of (identical) primitive cells (Fig. 1 shows two such identical cells). The Bloch basis state of energy \( E_\eta \) and wave vector \( K = K + G_{\eta} \), \( n = 0,1 \), is therefore written as

\[
|\psi_\eta(K + G_{\eta})\rangle = \sum_{m} \sum_{\alpha} \sum_{l=0}^{7} \frac{e^{iK_{R_m}}}{\sqrt{2N_S}} \delta^{(\alpha)} p^{(\alpha,\eta)}(K) |\alpha;X_{m,l,j}^{e}\rangle + G_{\eta} \exp(iK_{G_{\eta}}) \rho^{(\alpha)}(K)|\alpha;X_{m,l,j}^{e}\rangle.
\]

(17)

The factor of 2 in the square root occurs since there are two primitive cells per rectangular cell (see Fig. 1). The two-allowed values of \( G_{\eta} \) (there are two primitive cells per supercell) are given in Eq. (9).

At each supercell wave vector \( K \), there are \( 16N_{O,atom} \) supercell energy bands, while for a primitive cell, there are \( 8N_{O,atom} \) bands at each \( K = K + G_{\eta} \), \( n = 0,1 \). Each supercell state is thus a linear combination of all of the primitive-cell states:

\[
|\Psi_p(K)\rangle = \sum_{\eta=1}^{N_{O,atom}} \sum_{\alpha} \sum_{n=0}^{1} a_{\eta;\alpha,n} |\psi_\eta(K + G_{\eta})\rangle.
\]

(18)

Taking the inner product of Eq. (18) with \( \langle \alpha;X_{m,l,j}^{e}\rangle \) and employing Eqs. (14) and (15) result in a pair of equations for each atom-orbital pair \( (\alpha, j) \), \( \alpha = 1, \ldots, N_{O,atom} \), \( j = 0, \ldots, 7 \):

\[
\exp[-i(K \cdot p + K_d(\Delta_{\alpha}^{(j)}))] B_{p}^{(\alpha,j)}(K) = \frac{1}{\sqrt{2}} \sum_{\eta=1}^{N_{O,atom}} \sum_{n=0}^{1} e^{iG_{\eta} \cdot p} a_{\eta;\alpha,n} C_{p}^{(\alpha,j)}(K).
\]

(19)

In matrix form, these equations read

\[
B_{p}^{(\alpha,j)}(K) = U \cdot C_{p}^{(\alpha,j)}(K),
\]

(20)

where

\[
B_{p}^{(\alpha,j)}(K) = \begin{bmatrix} e^{-iK \cdot p} \rho_{0,p}^{(\alpha,j)}(K) \\ e^{-i(K + K_d(\Delta_{\alpha}^{(j)}))} \rho_{1,p}^{(\alpha,j)}(K) \end{bmatrix}, \quad C_{p}^{(\alpha,j)}(K) = \begin{bmatrix} \sum_{\eta=1}^{N_{O,atom}} a_{\eta;\alpha,n} C_{p}^{(\alpha,j)}(K + G_{\eta}) \end{bmatrix},
\]

(21)

and the unitary matrix \( U \) is

\[
U = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ e^{-iG_{1} \cdot p} & e^{iG_{1} \cdot p} \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.
\]

(22)

As in Refs. 3 and 5, Eq. (22) is solved repeatedly for each atom-orbital pair \( (\alpha, j) \), \( \alpha = 1, \ldots, N_{O,atom} \), \( j = 0, \ldots, 7 \), and the results are saved. Taking advantage of the normalization of the Bloch states yields the following relation:

\[
P_{p,n} = \sum_{\eta=1}^{N_{O,atom}} |a_{\eta;\alpha,n}|^2 = \sum_{\eta=1}^{N_{O,atom}} \sum_{j=0}^{7} |C_{p}^{(\alpha,j)}(K + G_{\eta})|^2,
\]

(23)

where \( P_{p,n} \) represents the probability that the supercell state \( p \) projects onto the primitive-cell states of wave vector \( K = K + G_{\eta} \), \( n = 0,1 \).

The probabilities \( P_{p,n} \) are computed and saved for all supercell states \( p \) and all primitive-cell states of wave vector \( K = K + G_{\eta} \), \( n = 0,1 \). The resulting (energy) spectrum at fixed wave vector \( K = K + G_{\eta} \), \( n = 0,1 \), is used in band determination. For a perfect structure such as the superlattice unfolded here, when primitive-cell bands for a given \( K \) are not degenerate (or nearly degenerate), each \( P_{p,n} \) projects onto a single primitive-cell state.8 For alloys or other imperfect structures, at a fixed \( K \), the \( P_{p,n} \) typically forms peaks around energies which represent the approximate primitive-cell bands, and the resulting steplike cumulative probability function can be used in approximate band definition.5

### III. RESULTS

The SiGe SL is modeled using the \( sp^3d^5s^* \) empirical tight-binding approach.8 The Si and Ge bulk parameters are taken from our earlier work.9 The two-center integrals for a Si-Ge nearest-neighbor pair have been optimized using our genetic algorithm10 to give the best \( \text{Si}_0.5\text{Ge}_0.5 \) bulk behavior within the virtual crystal approximation and are shown in Table I. Strain is present in the SL and alters both the two-center integrals and the on-site parameters. The two-center integrals are scaled using the customary generalization of Harrison's11 \( d^2 \) scaling law: \( U = U_0(d^2/d_0)^{\eta} \), where \( U_0 \) is an ideal two-center integral and \( d_0 \) and \( d \) are the ideal and actual bond lengths, respectively. The on-site parameter shifts are determined using our method presented in Ref. 12. The scaling exponents and shift constants are given in Tables II and III.

The behavior of the bulk Si and Ge band edges under biaxial and hydrostatic strain is shown in Figs. 4–7. For the
TABLE I. Nearest-neighbor two-center integrals for Si-Ge bonds (in eV).

<table>
<thead>
<tr>
<th>Two-center integral</th>
<th>Value (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ssσ</td>
<td>-1.574309</td>
</tr>
<tr>
<td>s*σ</td>
<td>-3.999753</td>
</tr>
<tr>
<td>s(Si)s'(Ge)σ</td>
<td>-1.440045</td>
</tr>
<tr>
<td>s(Ge)s'(Si)σ</td>
<td>-1.499091</td>
</tr>
<tr>
<td>s(Ge)p(Si)σ</td>
<td>2.760826</td>
</tr>
<tr>
<td>s(Si)p(Ge)σ</td>
<td>2.878285</td>
</tr>
<tr>
<td>s'(Ge)p(Si)σ</td>
<td>2.814474</td>
</tr>
<tr>
<td>s'(Si)p(Ge)σ</td>
<td>2.747303</td>
</tr>
<tr>
<td>s(Ge)d(Si)σ</td>
<td>-2.595310</td>
</tr>
<tr>
<td>s(Si)d(Ge)σ</td>
<td>-2.471630</td>
</tr>
<tr>
<td>s'(Ge)d(Si)σ</td>
<td>-1.029594</td>
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<tr>
<td>ppσ</td>
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<tr>
<td>ppτ</td>
<td>-1.626914</td>
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<tr>
<td>p(Ge)d(Si)σ</td>
<td>-2.022367</td>
</tr>
<tr>
<td>p(Si)d(Ge)σ</td>
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<tr>
<td>p(Ge)d(Si)π</td>
<td>2.504041</td>
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<td>p(Si)d(Ge)π</td>
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<tr>
<td>dστ</td>
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<tr>
<td>ddσ</td>
<td>2.501057</td>
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<tr>
<td>ddδ</td>
<td>-1.777856</td>
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</table>

TABLE II. Scaling exponents η (dimensionless) and unstrained lattice constants a₀ (nm) for two-center integrals between Si-Si, Ge-Ge, and Si-Ge.

<table>
<thead>
<tr>
<th></th>
<th>Si</th>
<th>Ge</th>
<th>Si-Ge</th>
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<tbody>
<tr>
<td>η</td>
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<td></td>
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<tr>
<td>ssσ</td>
<td>0.56247</td>
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<tr>
<td>s'σ</td>
<td>0.19237</td>
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<td>sσ</td>
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<td>spσ</td>
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<td>s'pσ</td>
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<tr>
<td>s'dσ</td>
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<td>1.831938</td>
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<tr>
<td>s'σdσ</td>
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<td>ppσ</td>
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<td>pdσ</td>
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<td>ddτ</td>
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<tr>
<td>ddδ</td>
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<td>3.06253</td>
<td>1.805441</td>
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<tr>
<td>a₀</td>
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<td>0.565790</td>
<td>0.554443</td>
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TABLE III. On-site parameter shift constants (dimensionless) and downward atomic shifts, Eₘₐₜ (in eV, same for both atoms) for orbital pairs Si-Si, Ge-Ge, and Si-Ge.

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<thead>
<tr>
<th></th>
<th>Si</th>
<th>Ge</th>
<th>Si-Ge</th>
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</thead>
<tbody>
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<td>ss</td>
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<td>0.00000</td>
<td>ss</td>
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<tr>
<td>s*σ</td>
<td>0.77849</td>
<td>6.28624</td>
<td>s'Sσ</td>
</tr>
<tr>
<td>s'(Si)s'(Ge)σ</td>
<td>1.78613</td>
<td>1.86887</td>
<td>s(Si)s'(Ge)σ</td>
</tr>
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<td>sp</td>
<td>0.48057</td>
<td>2.03278</td>
<td>s(Ge)p(Si)σ</td>
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<td>s'pσ</td>
<td>3.59244</td>
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<td>s'p(Ge)p(Si)σ</td>
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<td>0.16396</td>
<td>s(Ge)d(Si)σ</td>
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<tr>
<td>s'dσ</td>
<td>0.34243</td>
<td>1.98112</td>
<td>s'(Ge)d(Si)σ</td>
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<tr>
<td>p</td>
<td>4.07053</td>
<td>0.42830</td>
<td>p</td>
</tr>
<tr>
<td>pd</td>
<td>0.00000</td>
<td>0.12084</td>
<td>p(Ge)d(Si)σ</td>
</tr>
<tr>
<td>dd</td>
<td>5.30270</td>
<td>3.85908</td>
<td>dd</td>
</tr>
</tbody>
</table>

biaxial strain and SL calculations, the z-lattice constant was determined using the Keating model, with (α₃, β₃) = (48.5, 13.8), (α₃, β₃) = (39.0, 12.0) N/m; for the SL, α₃ = α₃. The valence band maxima of both materials and the X-valley conduction-band minima of Si and the L-valley minima of Ge were optimized to reproduce the predictions of van de Walle's model solid theory. The split-off holes were...
not strongly weighted in the optimization, however. The un-
optimized biaxial strain behaviors of the Ge-$X_x$, minima and
the Si-$L$ minima differ from van de Walle’s predictions\cite{14} and
are, in fact, closer to the behavior predicted by the pseudo-
potential calculations of Fischetti and Laux.\cite{15} For both hy-
drostatic and biaxial strains, there is a fairly wide variation in
the calculated behavior in the literature\cite{18}. See Refs. 14–17.

Figure 8 shows our calculation of the bands along [100]
for the Si(4)Ge(4) SL discussed above. The bands were un-
folded using the method of Sec. II from calculations based
on the rectangular cell of Fig. 2, which has two nonidentical
primitive cells. The Lanczos method\cite{18} was used to calculate
the eigenvectors, and an especially stringent minimum band
probability\cite{5} of 90\% was used in the zone-unfolding calcula-
tion, except at the highly degenerate folding point corre-
sponding to $k=(\pi/a_x)e_x$. (At points of high degeneracy, of-
ten only one of a pair of degenerate eigenvectors is returned
by the Lanczos method,\cite{18} so a lower criterion of 50\% was
used.) Note that the resolution is very good. Our calculations
give a minimum (indirect) gap of 0.825 eV and a minimum
direct gap of 1.048 eV; the next-higher direct gaps are 1.099,
1.728, and 1.743 eV. The experiments of Pearsall\ et\ al.\cite{6}
measured a minimum gap of 0.76 eV, with next-
higher gaps of 1.25, 2.31, and 2.58 eV. The LMTO calcula-
tions by Ikeda\ et\ al.\cite{7} found a minimum direct gap of about
1.27 eV, with next-higher direct gaps of 1.28, 1.66, and

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{Fig5}
\caption{Biaxial strain behavior of Si using our parameter set
(open symbols) and the model solid theory of Ref. 14 (solid sym-
bols). $X$ denotes $X$-valley minima, which generally occur a little
away from the symmetry point.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{Fig6}
\caption{Hydrostatic strain behavior of Ge using our parameter
set (open symbols) and the model solid theory of Ref. 14 (solid
symbols). $X$ denotes $X$-valley minima, which generally occur a little
away from the symmetry point.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{Fig7}
\caption{Hydrostatic strain behavior of Si using our parameter set
(open symbols) and the model solid theory of Ref. 14 (solid sym-
bols). $X$ denotes $X$-valley minima, which generally occur a little
away from the symmetry point.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{Fig8}
\caption{Unfolded bands along [100] for the Si(4)Ge(4) SL. The
bands were unfolded using the method presented here from calcu-
lations employing the rectangular cell of Fig. 2, which has two
nonidentical primitive cells.}
\end{figure}
1.68 eV in their ideal interface model, for their diffuse interface model, the minimum direct gap is about 1.04 eV. Although our lowest direct gap is smaller than that of Ikeda et al., it does not by itself account for the observed 0.76 eV transition, whose exact nature remains unresolved.

IV. CONCLUSIONS

We have shown that zone unfolding is possible even when the nonprimitive unit cell contains primitive cells which are not equivalent. We have shown how the allowed wave vectors must be chosen and have modified our zone-unfolding method to implement this process. We have used this modified method to unfold the bands of a Si(4)/Ge(4) SL studied both experimentally and theoretically and have achieved results in general agreement with earlier work. In addition, we give strain parameters for bulk Si and Ge and both two-center integrals and strain parameters for Si-Ge nearest-neighbor pairs in the \( sp^3d^5s^* \) empirical tight-binding approach. Because our modified method gives primitive-cell dispersion relations from nonprimitive rectangular cells with nonequivalent primitive cells, general nanodevice simulation tools become simpler to construct. A set, easily programed rectangular cell can be used, and the method presented here can still unfold the true primitive-cell \( E(k) \) relations.

ACKNOWLEDGMENTS

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2 NEMO3D development is being continued by the Network for Computational Nanotechnology (NCN). Simulations were performed on nanoHUB.org resources. nanoHUB.org is a web site dedicated to advancing nanotechnology through theory, modeling, and simulation for research and education.


18 G. H. Golub and C. F. van Loan, Matrix Computations (Johns Hopkins University Press, Baltimore, 1989), Chap. 9