# Direct-gap Si/Ge superlattices

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Theoretical predictions of electronic and optical properties of short-period Ge-rich Si/Ge superlattices are used to demonstrate that the problem of obtaining direct-gap Si-based structures is best addressed from the point of view of removing the indirectness of Ge with biatomic sheets of Si. The concept of a buffer-induced optical window is proposed.

Since the pioneering calculations of Gnutzmann and Clausecker,[1] there has been considerable speculation on the possibility of creating artificial Si-based crystals with a direct gap. A stimulus to intensifying activities towards realization of this goal has come with advances in Si/Ge molecular-beam epitaxy and with the first observation of optical transitions in Si/Ge short-period superlattices.[2] However, all Si/Ge structures that have been discussed in the literature so far have been indirect. Si-based structures with a direct gap have remained elusive. In this paper, electronic and optical properties of a representative sequence of short-period Ge-rich Si/Ge superlattices are presented which demonstrate for the first time the existence of direct-gap Si-based structures.

The method used to calculate electronic and optical properties of these short-period structures involves the use of empirical pseudopotentials with spin-orbit coupling.[3] Parameters used in the calculations have been given elsewhere in connection with a study of the Si/Ge (4:4) superlattice (SL).[4] The notation used in Ref. 4 is also used here to specify a particular SL. The term $(M{:}N)$ is used to denote a Si/Ge(001) SL in which the Si layer consists of $M$ atomic monolayers and the Ge layer consists of $N$ atomic monolayers, stacked in the [001] direction. The offsets used in the calculations are those given by Van de Walle and Martin.[5]

The representative sequence of regular SL's considered in this study is one in which the width of the Si layer is fixed at $M=2$ and the width of the Ge layer takes the values $N=2(2n+1)$, with $n=0,1,2,3,4,5$. This representative sequence is taken from the set of $(2{:}N)$ structures, which have space groups $D_{2h}^{5}$, $D_{2h}^{28}$, and $D_{4h}^{19}$. These structures are centrosymmetric. The notation used in Ref. 4 to label the SL states is also used here; in particular, the labels $V1$ and $C1$ are used to denote the uppermost valence state and the lowest conduction state, respectively. In the present work, $P$ is defined as $\log_{10}$ of the sum over spin of the modulus squared of the dipole matrix element $M=\langle \psi_{\text{val}}|\hat{\mathbf{e}}\cdot\mathbf{p}|\psi_{\text{cond}}\rangle$ for an optical transition between two SL states. The notation used is such that $z$ denotes the polarization component perpendicular to the interfaces, and $x$-$y$ denotes the sum of the $x$ and $y$ components.

In Fig. 1, values of $P$ with $x$-$y$ and $z$ polarization for the $V1$-$C1$ zone-center transition are shown for the cases of the Si/Ge $[(2{:}N);\ N=2,6,10,14,18,22]$ SL's grown on Si(001) and Ge(001). The fact that the SL's on Si(001) other than the (2:2) and perhaps the (2:6) SL cannot be grown in practice, owing to difficulties with critical thickness,[2] is not relevant to the present study. These particular results are presented in order to make a comparison with the Ge(001) results; the superlattices on Ge(001) can be grown, albeit to limited thickness. The results presented in Fig. 1 have been obtained with a heterointerface spacing between the Si and Ge layers given by $d=\frac{1}{8}[A(\text{Si})+A(\text{Ge})]$, where $A$ is the cubic lattice constant.[4] Uncertainties in the heterointerface spacing do not affect the conclusions of this work regarding possibilities for direct-gap structures. It can be seen from Fig. 1 that the $P$ values are generally within 4 orders of magnitude of the $P$ value (denoted as $P'$) for a good direct transition, which in the units of Fig. 1 would have a value of approximately $-0.4$.[6] In some cases the $P$ value is only a factor of about 2 lower than $P'$.

In the case of the (2:2) and (4:4) superlattices on Si(001), the $P(x\text{-}y)$ values for the lowest-energy dipole-allowed cross-gap transition at the zone center are calculated to be $-1.7$ and $-2.7$,[4] respectively. Since the corresponding quantities calculated within the local-density approximation are $-1.8$ and $-3.2$,[7] it is assumed that the validity of the empirical-pseudopotential method is not in question for the structures considered in this paper.

It has been shown for the case of the (4:4) SL that a

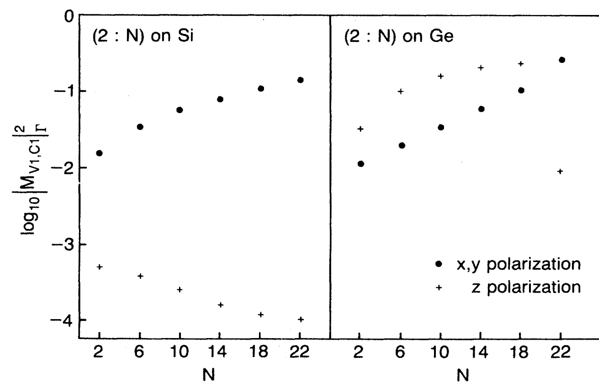


FIG. 1. Plots of $P$ for the zone-center $V1$-$C1$ transition with $x$-$y$ and $z$ polarization in the Si/Ge $[(2{:}N);\ N=2(2n+1),\ n=0,1,\ldots,5]$ superlattices on Si(001) and Ge(001). The superlattices grown on SiGe have intermediate $P$ values.

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hole reversal is induced with an increasing percentage of Ge in the SiGe buffer.[4] The effect of hole reversal can be seen in the inversion between substrates of the polarization dependence of the $P$ values shown in Fig. 1. For the case of the Si substrate, the uppermost SL valence state is an $m_j=\frac{3}{2}$ state. This is reflected in the substantial optical anisotropy exhibited by the SL's grown on Si. As the width of the Ge layers is increased from 2 to 22, the optical anisotropy increases as a result of diminishing light-hole admixture into state $V1$.

For the case of the Ge substrate, the uppermost valence state is, for $N<22$, basically an $m_j=\frac{1}{2}$ state, although substantial heavy-hole–light-hole mixing is present. Hole reversal (or partial hole reversal) is reflected in the fact that the transitions with $z$ polarization have higher $P$ values compared with the transitions with $x$-$y$ polarization. As $N$ is increased from 2 to 18, the optical anisotropy is reduced and the $P(x\text{-}y)$ and $P(z)$ values approach $P'$. This can be understood in terms of the complete SL-buffer system beginning to resemble a cubic Ge crystal with only the ultrathin sheets of Si taking up the strain. The presence of the biatomic sheets of Si is crucial in removing the inherent indirectness of bulk Ge due to the $L$ valleys. As the thickness of the Ge layers is further increased, it is expected that the uppermost heavy-hole state would be pushed closer to the band edge of Ge than the uppermost light-hole state (the Ge layers are not under tetragonal distortion, and so the top of its valence band is not strain split). Thus, reversion to the hole alignment present in the Si-buffered structures, concomitant with increased polarization anisotropy, is expected as $N$ is increased. Such a feature is apparent at $N=22$ on the right-hand side of Fig. 1.

The charge density of the lowest conduction state (state $C1$) at the zone center of the (2:18) SL on Si is shown in Fig. 2. In this figure the Si atomic sites are indicated by circles and the Ge atomic sites by squares. It can be seen from this figure that state $C1$ has considerable tunneling amplitude in the Ge regions as a result of the momentum mixing that is occurring.[4] The orthogonalization mechanism[8] is essentially independent of the distribution of strain within the unit cell.

Since the optical dipole matrix elements reflect the momentum mixing occurring in the superlattice, strong candidates for direct-gap behavior can be identified from evaluation of an integral of the product of the wave functions (viewed as tunneling states) associated with the $\Gamma$ and $X$ points multiplied by the deviation of the superlattice potential from the virtual crystal potential. Since the wave function product changes sign from one unit cell to the next, promising structures turn out to be those with $M=2$. However, the trends shown in Fig. 1 indicate that second-order processes, which participate coherently, also play an important role.

Detailed investigations of the properties of the (4:4) SL have shown that as the amount of Ge in the buffer layer is increased, the zone-edge conduction states associated with the [100] and [010] directions are driven up past the lowest zone-center conduction state.[4] Once this channel for indirectness has been removed, it is still necessary, in order to verify that a SL may be inherently direct, to es-

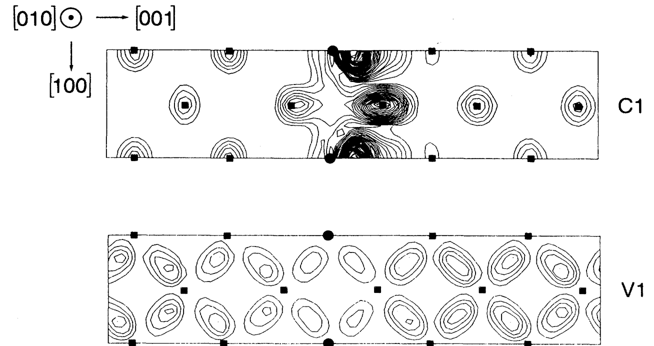


FIG. 2. Charge densities (with contour spacings of 0.5 a.u.) of state $C1$ and $V1$ at the zone center of the Si/Ge (2:18) superlattice on Si(001). The maximum charge densities shown are 15 for $S1$ and 2 for $V1$.

tablish that the lowest zone-center conduction level represents the global minimum in the conduction band. This is, in fact, the case for the $(M:N)$ SL's considered here, apart from the (2:2) SL, which has a longitudinal dispersion in $C1$ which always renders the SL indirect and the SL's with $N \gtrsim 12$ which are indirect through $L$-related states. For example, in the (2:6) SL, state $C1$ disperses upwards in going out along $k_z$ from the zone center to the zone edge.[5] The crossover of the transverse

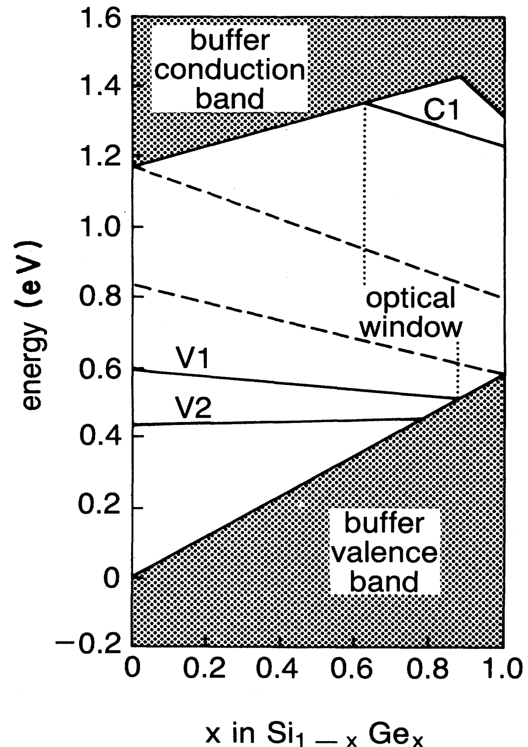


FIG. 3. Energies of zone-center states $V1$, $V2$, and $C1$ in the (2:6) SL grown on SiGe(001) buffers. Also shown are the band edges of the buffer (shaded region) and the bulk edges (dashed lines) associated with the Si and Ge layers making up the SL. The optical window for quasidirect transitions between $V1$ and $C1$ lies approximately in the buffer range 60–90 at. % Ge.

state $C1$ and the zone-center level occurs with a SiGe buffer composition of about 83%:17%. Thus, the (2:6) [and the (2:10), etc.] SL is inherently direct only when grown on buffers containing more than about 20% Ge. The fact that state $C1$ in most Si/Ge SL's disperses downwards along $k_z$ is a reflection of the complicated form of the bulk conduction-band minima lying along the $\Delta$ line.

Having established the inherent directness of a SL, it is necessary to ensure directness of a complete SL-buffer system; this point is intimately connected with the problem of band offsets.[5] In the case of a Si buffer, the lowest conduction states in the SL-buffer system are the bulk $\Delta$ conduction states in the Si layers cladding the SL, whereas the uppermost valence states are the valence states in the SL. The SL-buffer system is indirect in real space, irrespective of the indirectness already inherent in the SL.

The alignment giving rise to indirectness is reversed in the case of a Ge buffer. The lowest conduction state [for the (2:6), etc. SL's] is the SL state $C1$ at the zone center, whereas the uppermost valence states are the bulk zone-center states in the Ge layers cladding the SL. Changing the compositions of (Ge-rich) alloy layers cladding (sequences of) Si/Ge SL's provides scope for manipulating the alignments. We focus on the (2:6) SL.

In Fig. 3 the zone-center superlattice states ($V2$, $V1$, and $C1$) closest to the band edges are plotted together with the band edges of the buffer and the band edges (which are nonallowed levels within this system) associated with the Si and Ge layers making up the SL. It can be seen from Fig. 3 that zone-center transitions between SL states $V1$ and $C1$ can take place readily only within a restricted range (between about 60 and 90 at. % Ge) of buffer compositions. However, for the (2:6) SL it is, in any case, most appropriate to grow on Ge-rich (75 at. % Ge) buffers in order to achieve strain symmetrization[9] and so avoid limitations on SL thickness. Properties of these direct and various other Si/Ge SL's will be described in detail elsewhere.[10]

In summary, it has been shown that the problem of obtaining direct-gap Si-based structures is best addressed from the point of view of removing the indirectness of Ge with biatomic sheets of Si, and the concept of a buffer-induced optical window has been proposed. Experimental verification of the important theoretical predictions (energy levels, matrix elements, polarization effects, optical windows) made here is called for.

*Notes added in proof.* Friedel and co-workers [P. Friedel, M. S. Hybertson, and M. Schlüter, Phys. Rev. B **39**, 7974 (1989)] have performed empirical pseudopotential calculations on the (2:2) superlattice and also found good agreement with results from first-principles calculations. This is in spite of the fact that the superlattice layers are only two atoms in thickness and so any atomic sheet has atomically dissimilar neighbors.

After this work was first submitted, Satpathy and coworkers [S. Satpathy, R. M. Martin, and C. G. Van de Walle, Phys. Rev. B **38**, 13 237 (1988)] proposed that the (4:6) and (3:7) superlattices should be direct-gap superlattices. These structures have squared optical dipole matrix elements at the zone center which are at least 1 order of magnitude lower than those considered in the present study. Also, the concept of an optical window applies to these structures.

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[5]C. G. Van de Walle and R. M. Martin, Phys. Rev. B **34**, 5621 (1986).

[6]For example, the sum over spin of $|M|^2$ for the $\Gamma_8^V$-$\Gamma_6^C$ transition in bulk GaAs is calculated to be 0.446 a.u., giving a value of $P=-0.35$. Thus, the value of $E_P$ [P. Lawaetz, Phys. Rev. B **14**, 3460 (1971); $E_P=25.7$ eV] is calculated to be 24.3 eV.

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