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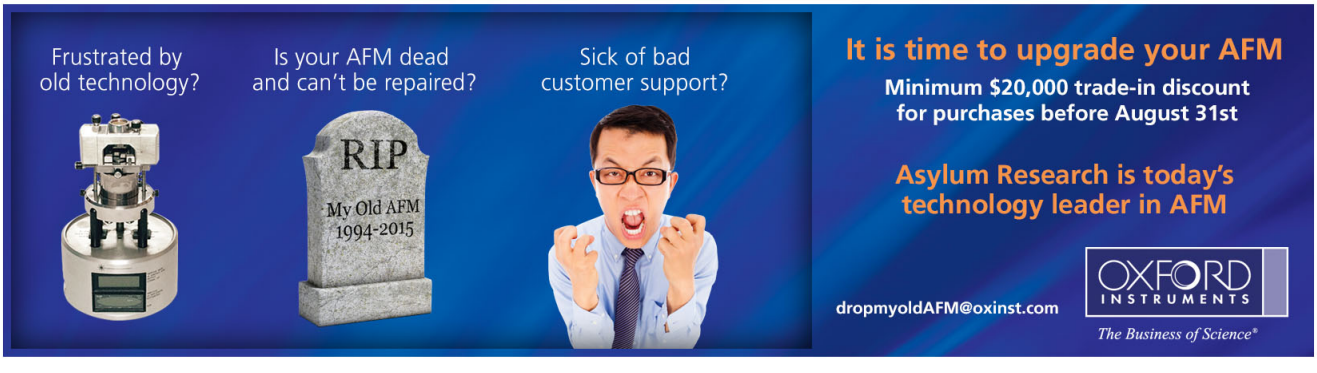

Electronic structure of [110] Si-Ge thin-layer superlattices

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First-principles electronic structure calculations for Si_nGe_n superlattices (for $n = 4$, 6, and 8) grown epitaxially on a (110) Si substrate reveal a nearly direct band gap (to within $\approx$0.04 eV for $n = 4$) despite the pronounced indirectness of its constituents. This is unlike superlattices grown in the [001] direction, which are indirect when grown on Si and quasi-direct only on substrates with larger lattice constants, e.g., Ge. Transition dipole matrix elements for the lowest energy direct transition vanish for all repeat periods n but are finite for several other new low-energy transitions.

When the atoms in a disordered alloy are arranged into the ordered structure of a superlattice, the original alloy Brillouin zone folds into a smaller superlattice zone. This folding can convert indirect transitions in the alloy into direct, optically allowed transitions in the superlattice. This possibility has spurred current interest in thin-layer superlattices of Si and Ge,[1–10] where two indirect, technologically mature constituents can potentially be grown as a direct band gap compound using molecular beam epitaxy. So far, the research has focused on [001] oriented substrates and superlattices. These have been predicted[3,5,6] to be quasi-direct[11] (at $\bar{\Gamma}$) when grown on Si-Ge alloy (with at least 50% Ge content) or Ge substrates,[9,10] but are indirect when grown on Si.[3,5,6,8] For such [001] superlattices, band states along the [001] Δ direction fold to $\bar{\Gamma}$. Substrate-induced tetragonal deformation of the superlattice splits the degeneracy of the six X conduction-band minima and for Ge substrates causes the $\bar{\Gamma}$-folding [001] X state to fall below the nonfolding X states at [100] and [010]. The overall gap can therefore be direct. On Si substrates the reverse is true and the superlattices remain indirect.

Superlattices grown in the [110] direction also have an increased repeat period (with respect to fcc) along the [001] direction. Thus, in addition to points along the superlattice [110] Σ direction, the [001] X point folds to $\bar{\Gamma}$.[12] Unlike the [001] superlattices, the folding X point now has its k vector parallel to the substrate. This reverses the effect of substrate-induced strain on the order of folding versus nonfolding X states, and we may therefore also expect the effect of the substrate on the overall directness of the superlattice to be reversed. This raises the possibility of growing a direct band-gap Si-Ge superlattice on a Si substrate, provided it is grown in the [110] direction. To investigate this, we have performed self-consistent first-principles nonlocal pseudopotential calculations within the local density approximation (LDA) for Si_nGe_n [110] superlattices with $n = 4$, 6, and 8. The calculations are carried out as described in Ref. 6. All structural degrees of freedom have been relaxed subject to the constraint of coherent growth on Si. We find that all the [110] superlattices have the same total energy (to within 3 meV per Si-Ge pair), equal to the energy of the previously calculated [001] superlattices.[6] The LDA, with its well known band-gap problem, underestimates conduction-band energies. Fortunately, the lowest superlattice conduction bands derive only from Si and Ge X states. We can therefore approximately correct for the LDA error, at least for the X-derived states, by shifting our calculated conduction-band states upwards by 0.64 eV, as discussed in Ref. 6.

Figure 1 shows calculated band energies at symmetry points for the $n = 4$,6, and 8 [110] superlattices. We also show (as $n = \infty$) values appropriate for a Si/Ge interface, i.e., calculated band offsets. We calculate an average valence-band offset for the Si-Ge interface of 0.5 eV. The band energies of each superlattice have been appropriately aligned so that any band offset can be read off the figure. Figure 2 shows planar-averaged wave functions $|\psi|^2$ for the $\bar{\Gamma}$-folding

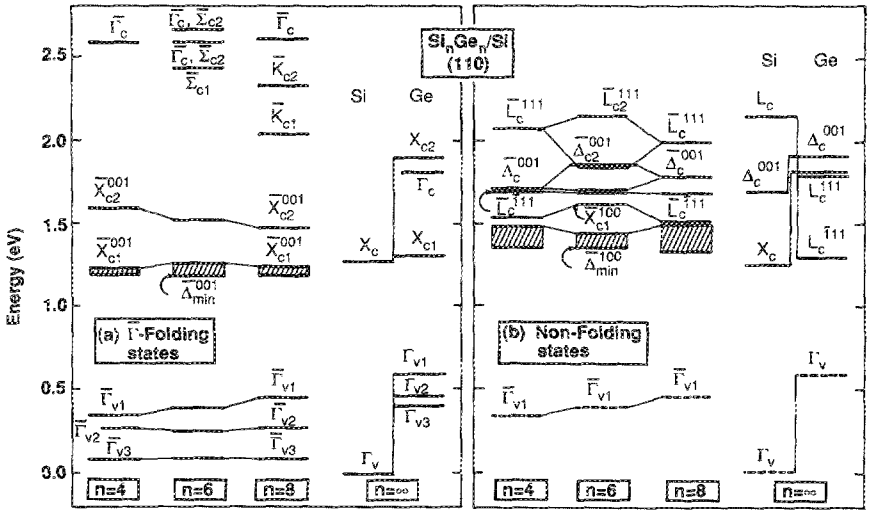

FIG. 1. Energy levels (in eV) of (a) $\bar{\Gamma}$-folding states and (b) nonfolding states for strained [110] Si_nGe_n superlattices grown on Si for $n = 4$, 6, and 8 and for the superlattice constituents Si and Ge on Si (in columns as indicated). The shaded boxed regions indicate the extent of downward dispersion of a band away from the symmetry point. The energy levels for the different superlattices have been aligned using calculated band offsets and the conduction-band energies have been shifted 0.64 eV upwards to approximately correct for LDA errors.

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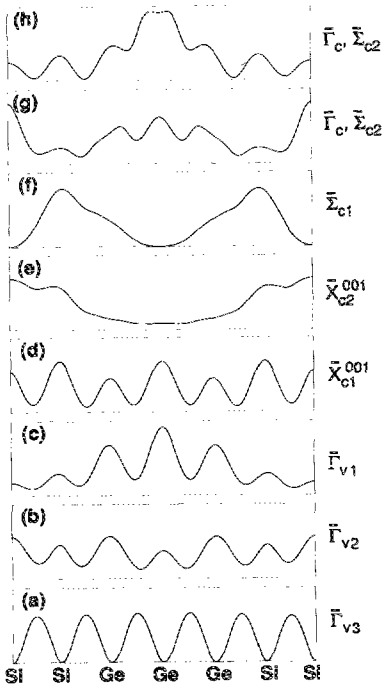

FIG. 2. (110) planar averaged wave functions for $\bar{\Gamma}$-folding states in the Si_6Ge_6 superlattice. The states are sorted with respect to energy (a–h) with symmetry as indicated.

states in the $n = 6$ superlattice. We have chosen to label the states with fcc symmetry labels indicating the alloy origin of each state and adding an overbar to indicate that it is a superlattice state.

Figure 1(a) shows the energies of states that fold to the center of the superlattice zone, $\bar{\Gamma}$. The valence-band maximum is located here and is formed from the alloy Γ'_{25} p states. They are split into $\bar{\Gamma}_{v1}$, $\bar{\Gamma}_{v2}$, and $\bar{\Gamma}_{v3}$ by substrate-induced strain and interaction with folded-in states of the same symmetry. The uppermost valence-band state, $\bar{\Gamma}_{v1}$, is localized on the Ge sublattice [see Fig. 2(c)] and its energy approaches the Ge valence-band edge as the superlattice thickness increases. The lowest conduction band at $\bar{\Gamma}$, $\bar{X}^{001}_{c1}$, is formed by a folded-in [001] X state. The symmetry of this state (see Table I) changes with n, causing a small shift upwards for $n = 6$ as it interacts with the valence-band state $\bar{\Gamma}_{v2}$. This is also seen in the complementary nature of the wave functions [see Figs. 2(b) and 2(d)]. There is a small residual downward dispersion immediately away from $\bar{\Gamma}$, reflecting the downward dispersion from X to the conduction-band minimum at Δ in the alloy. This dispersion is indicated by the shaded area in Fig. 1(a), and amounts to 35, 72, and 50 meV for $n = 4$, 6, and 8, respectively. For comparison, the dispersion of the folded-in [001] X states in [001] oriented superlattices is 99, 85, and 13 meV for $n = 2$, 4, and 6 grown on Si[5] and 114 meV for the $n = 4$ superlattice grown on Ge.[6] The folding of states along the superlattice direction Σ does not lead to low-energy states until $n = 6$, when a point close to K folds, and $n = 8$, when the K point itself folds. For $n = 6$, the folding state labeled $\bar{\Sigma}_{c2}$ interacts strongly with the original alloy Γ_2 state (both of B_{1u} symmetry), making identification of their origins in alloy states impossible. The $\bar{\Gamma}$-folding conduction-band states are delocalized with the exception of the $\bar{X}^{001}_{c2}$ state, which is localized on the Si sublattice, and the upper of the $\bar{\Gamma}_c$,$\bar{\Sigma}_{c2}$ pair, which is localized on the Ge sublattice [see Figs. 2(e) and 2(g)].

TABLE I. Symmetry labels for $\bar{\Gamma}$-folding states with point group symmetry *mmm*. The symmetry notation is from Tinkham, *Group Theory and Quantum Mechanics* (McGraw–Hill, New York, 1964).

State	Symmetry $n = 4$	$n = 6$	$n = 8$
$\bar{\Gamma}_c$	B_{1u}	B_{1u}	B_{1u}
$\bar{\Sigma}_{c2}$,$\bar{K}_{c2}$		B_{1u}	B_{2g}
$\bar{\Sigma}_{c1}$,$\bar{K}_{c1}$		B_{2g}	B_{1u}
$\bar{X}^{001}_{c2}$	B_{2g}	B_{1u}	B_{2g}
$\bar{X}^{001}_{c1}$	B_{3u}	A_{1g}	B_{3u}
$\bar{\Gamma}_{v1}$	B_{3g}	B_{3g}	B_{3g}
$\bar{\Gamma}_{v2}$	A_{1g}	A_{1g}	A_{1g}
$\bar{\Gamma}_{v3}$	B_{2g}	B_{2g}	B_{2g}

Low-energy nonfolding states are shown in Fig. 1(b). These are derived from the various alloy Δ, X, and L points and are labeled accordingly. $\bar{\Delta}^{100}_{\min}$ is the conduction-band minimum along [100] and [010] directions and $\bar{\Delta}^{001}_{c1}$ and $\bar{\Delta}^{001}_{c2}$ are states folded from $[001]\,\pi/a$. Comparing Figs. 1(a) and 1(b) we see that the $\bar{\Gamma}$-folding [001] $\bar{X}^{001}_{c1}$ state is indeed below all nonfolding $\bar{X}$, $\bar{\Delta}$, and $\bar{L}$ states. The downward dispersion immediately away from $\bar{\Gamma}$ still leaves the superlattice indirect, but its small magnitude (35 meV for $n = 4$) makes this superlattice quasi-direct[11] at room temperature.

Our calculation does not include spin-orbit coupling, although qualitative features can be estimated from perturbation theory.[13] Its main effect is to couple the top three states, $\bar{\Gamma}_{v1-3}$, at the valence-band maximum. This can make dipole-forbidden transitions weakly allowed, and can shift the top valence-band state upwards by at most $\Delta_0/3$, where Δ_0 is the spin-orbit splitting at the valence-band maximum for the unstrained solid: 0.04 eV for Si, 0.30 eV for Ge, and $\approx$0.17 eV for the superlattices (the average of the constituents). This shift reduces the direct band gap and slightly modifies the valence-band offsets. The effect of spin orbit on the confinement of the superlattice states is thus expected to be small.

Table II shows calculated dipole matrix elements for the $\bar{\Gamma}$-folding states up to and including the alloy Γ state at $\approx$2 eV. Matrix elements for transitions to states folded from the [001] X point are smaller than those folded from the Σ or K points and are much smaller for $n = 4$ and 8. This can be understood by considering the orientation dependence of the ordering potential: the difference between the potentials of the ordered superlattice and of the disordered alloy after planar averaging in a given direction. Assigning constant potentials V_{Si} to the Si layers and V_{Ge} to the Ge layers, we can approximate the ordering potentials as follows. In the [110] direction the ordering potential is simply the difference $V_{Si} - V_{Ge}$, independent of the repeat period. In the [001] direction, responsible for the folding of the [001] X point, the ordering potential is $2(V_{Si} - V_{Ge})/n$ for $n = 2$, 6, 10, etc., and zero otherwise. This explains the extraordinarily small matrix elements for $n = 4$ and 8, and why they are

TABLE II. Calculated transition energies ΔE and dipole matrix elements $|\langle i|\hat{e}\cdot\mathbf{p}|f\rangle|^2/m_e$, both in eV. Each transition has a nonzero dipole matrix element for the given polarization $\hat{e}$ only. The transition energies can be approximately corrected for LDA errors by adding 0.64 eV.

$\langle i\|$			Γ_{v1}			Γ_{v2}			Γ_{v3}	
n	$\|f\rangle$	ΔE	$\frac{\|\langle\hat{e}\cdot\mathbf{p}\rangle\|^2}{m_e}$	$\hat{e}$	ΔE	$\frac{\|\langle\hat{e}\cdot\mathbf{p}\rangle\|^2}{m_e}$	$\hat{e}$	ΔE	$\frac{\|\langle\hat{e}\cdot\mathbf{p}\rangle\|^2}{m_e}$	$\hat{e}$
	$\bar{X}_{c1}$	0.24	0.0		0.32	$2.1\ 10^{-4}$	[110]	0.50	3.3×10^{-4}	[001]
4	$\bar{X}_{c2}$	0.61	0.0		0.69	0.0		0.87	0.0	
	$\bar{\Gamma}_c$	1.60	2.1	[$\bar{1}$10]	1.68	5.4	[001]	1.86	12.0	[110]
	$\bar{X}_{c1}$	0.22	0.0		0.37	0.0		0.53	0.0	
	$\bar{X}_{c2}$	0.48	9.6×10^{-3}	[$\bar{1}$10]	0.63	$1.1\ 10^{-2}$	[001]	0.79	1.5×10^{-1}	[110]
6	$\bar{\Sigma}_{c1}$	1.39	0.0		1.54	0.0		1.70	0.0	
	$\bar{\Gamma}_c,\bar{\Sigma}_{c2}$	1.55	1.2	[$\bar{1}$10]	1.70	2.3	[001]	1.86	5.6	[110]
	$\bar{\Gamma}_c,\bar{\Sigma}_{c2}$	1.63	2.0	[$\bar{1}$10]	1.77	3.3	[001]	1.94	7.1	[110]
	$\bar{X}_{c1}$	0.15	0.0		0.33	$1.2\ 10^{-5}$	[110]	0.51	7.8×10^{-5}	[001]
	$\bar{X}_{c2}$	0.38	0.0		0.56	0.0		0.74	0.0	
8	$\bar{K}_{c1}$	0.94	1.0×10^{-1}	[$\bar{1}$10]	1.12	$2.9\ 10^{-1}$	[001]	1.31	7.1×10^{-1}	[110]
	$\bar{K}_{c2}$	1.23	0.0		1.41	0.0		1.60	0.0	
	$\bar{\Gamma}_c$	1.51	3.8	[$\bar{1}$10]	1.69	5.5	[001]	1.88	12.0	[110]

orders of magnitude larger for $n = 6$. Unfortunately, the lowest energy dipole transitions in the $n = 6$ superlattice are symmetry forbidden.

We have shown that thin-layer Si-Ge superlattices grown on Si substrates have quasi-direct band gaps provided they are grown in the [110] direction. The dipole matrix element for the lowest energy transition vanishes, but there are new low-energy optically allowed transitions with LDA corrected energies of 0.96 and 1.14 eV (for $n = 4$), 1.12, 1.27, and 1.43 eV (for $n = 6$), and 0.97 and 1.15 eV (for $n = 8$). The minimum indirect gaps are 0.74, 0.97 and 0.89 eV, respectively.

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[11]Quasi-direct implies that $\bar{\Gamma}$ is lower in energy than $\bar{X}$, but the superlattice is nevertheless indirect because of a small downward dispersion (of the order kT) of the lowest conduction band away from $\bar{\Gamma}$.

[12]This can also be seen by noting that the [001] X point can be found at $2\pi/a\times$[110] along the Σ direction. This point folds to $\bar{\Gamma}$ for all [110] superlattices.

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