Comment on "Electronic Structure and Optical Properties of Si-Ge Superlattices"

We have self-consistently calculated[1] the electronic structure of the strained Si_4Ge_4/Si(001) superlattice, interpreting the electroreflectance transitions[2] A (observed 1.24 eV, calculated 1.26 eV) and B (observed 1.8 eV, calculated 1.74 eV) as folded-in (pseudo) direct excitations [Figs. 1(a)-1(c)], in accord with Ref. 2. In contrast, transition I, observed at 0.8 eV and interpreted previously[2] as the *direct* band gap, was shown to be an indirect $\bar{\Gamma}_v \rightarrow \bar{\Delta}_c$ excitation either to the superlattice Δ_c state (calculated[1] at 0.92 eV) or to the substrate Δ_c state (calculated at 0.80 eV). Other calculations[3] and experiments[4] support this assignment. More recently, Wong *et al.*[5] carried out non-self-consistent calculations within the empirical pseudopotential method. The central point of their Letter was to note that if larger Ge-Ge interplanar spacings were postulated (making the Ge—Ge bond lengths longer and more bulklike), the direct superlattice band gap (transition A) was reduced from 1.2 to 0.9 eV, close to the value where transition I was seen.[2] On the basis of this empirical adjustment, they proposed that the observed[3] transition I is in fact the *direct* band gap (A), in conflict with more recent experiments.[4] This parameter adjustment was not constrained by any (variational or microscopic) principle; the only motivation was that it might mimic effects of defects at Si/Ge interfaces. However, such interfacial defects are more likely to destroy coherence with the substrate, removing the biaxial epitaxial constraint ($a_{\parallel} = a_{Si}$), than to permit uniaxial relaxation of Ge—Ge bonds. In both cases Ge—Ge bonds relax, but in the former the Ge-Ge interplanar distance naturally becomes *smaller.* We show below that (i) even if the assumed *increase* in Ge-Ge interplanar distances were correct, the results of Wong *et al.* lead to further inconsistencies with the data, and (ii) to make the system more nearly direct, one needs to *reduce* the Ge-Ge interplanar spacing.

The observations pertinent to the understanding of the direct and indirect gaps in this system are the following: (i) Strain splits the conduction band at X into $X_c^{\perp}$ and $X_c^{\parallel}$; the valence-band maximum at Γ splits into $\Gamma_v^{\perp}$ and $\Gamma_v^{\parallel}$ (here $\perp$ and $\parallel$ denote directions perpendicular and parallel to the interface, respectively). (ii) For compressive strain [a Si substrate, Figs. 1(a) and 1(b)], $X_c^{\parallel}$ is below $X_c^{\perp}$ and $\Gamma_v^{\perp}$ is below $\Gamma_v^{\parallel}$, but for tensile strain [a Ge substrate, Figs. 1(e) and 1(f)], $X_c^{\perp}$ is below $X_c^{\parallel}$ and $\Gamma_v^{\parallel}$ is below $\Gamma_v^{\perp}$. (iii) By symmetry, only $X^{\perp}$ folds into $\bar{\Gamma}$ for [001]-oriented superlattices.

When the Ge-Ge interplanar spacing is increased (by assumption[5]), the conduction-band ($X_c^{\perp} - X_c^{\parallel}$) and the valence-band-maximum ($\Gamma_v^{\parallel} - \Gamma_v^{\perp}$) splittings increase too. In the calculation of Wong *et al.*, $\Gamma_v^{\parallel}$ was raised by 0.3 eV more than $X_c^{\perp}$, reducing by this amount the energy of transition A. However, the same effect must also

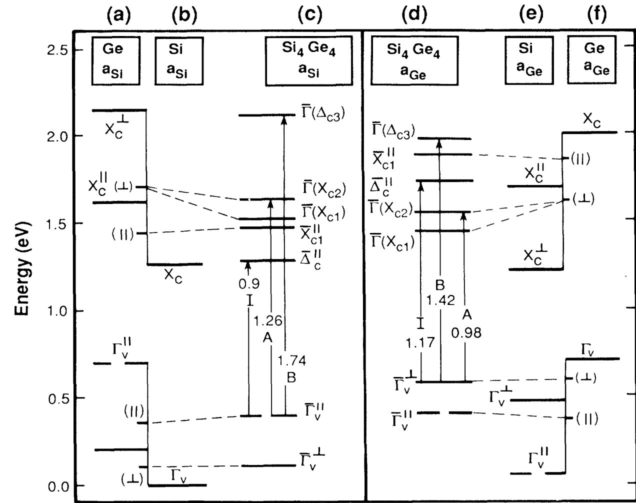

FIG. 1. Electronic energy levels for Si_4Ge_4 superlattice and its constituents on Si and Ge substrates. Band offsets are from Ref. 1.

reduce the energies of I ($\Gamma_v^{\parallel} - \Delta_c^{\min}$) and B [$\Gamma_v^{\parallel} - \bar{\Gamma}(\Delta_{c3})$] to below 0.8 eV and[5] to 1.4 eV, respectively. This creates a substantial conflict with the recently observed indirect transition (I) at 0.8 eV,[4] and fails to account for the pseudodirect transition (B) at[4] 1.8 eV. These are naturally interpreted within our model as transition I and B, respectively (calculated at ~0.8 and 1.74).

Our first-principles calculation [Figs. 1(d)-1(f)] shows that to make the system more nearly direct one needs to invert the order of $X_c^{\perp}$ and $X_c^{\parallel}$ and that this can be achieved by *reducing* the Ge-Ge interplanar spacing, *not* by increasing it.[5] The former condition is achieved on a Ge substrate [Fig. 1(d)], for which our calculation shows $I > A$. A similar trend is expected on a Si substrate when defects destroy coherence with the substrate.

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