

Invited

Electronic Structure of Ge-Si Atomic Layer Superlattices

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Strained-layer superlattices of Ge and Si with a period close to that of the fundamental unit cell of Si can be grown pseudo-morphically on Si substrates. We have examined such the energy-level structure of these superlattices by electro-reflectance spectroscopy. Our results show that the superlattice structure introduces a series of new energy levels not found in random alloys of the same average composition. This result has important implications for band-structure engineering of Ge-Si device structures. Prospects for constructing a direct bandgap Ge-Si semiconductor will be discussed.

Strained-layer epitaxy is a technique for growing lattice mismatched heterostructures without introducing, in principle, any additional defects from the lattice mismatch strain.^[1] We have examined structures of strained Ge grown on Si. In this case, the maximum permissible Ge-layer thickness is 6 atomic monolayers. Since this is rather thin, an extended structure may be built up by alternating atomic layers of Ge with atomic layers of Si. The presence of a relatively thick (400 μ m) Si substrate means that the strain in the Si epitaxial layers is negligible. Several repetitions of the Ge-Si structure are possible before the strain limit is again reached. The repeating structure forms a superlattice, and in this work we report our results on superlattices composed of alternating monolayers (1:1), bilayers (2:2) and 4-layers (4:4) of Ge and Si grown on [001] Si.^[2] These structures have a similar average composition that is: Ge_{0.5}Si_{0.5}. The energy-band structure of strained Ge-Si alloys is shown in Figure 1. This figure shows that direct band-to-band transitions for a strained Ge-Si alloy lie

above 2.5 eV while the indirect bandgap appears at 0.6 eV.^[3] The energy level spectra of Ge-Si atomic layer superlattices are shown in Figure 2. These spectra are taken using electro-reflectance spectroscopy at 300K.

The top-most spectrum show our results for a (1:1) atomic-layer superlattice. This spectrum shows prominent features at about 2.6 eV and 2.9 eV. Taking quantum confinement effects into account, these transitions coincide with those expected for the E₀ and E₁ transitions in a random alloy.^[4]

It is easily seen that the other two spectra in Figure 2 are more complex. The spectrum for the (2:2) superlattice shows a strong transition at 2.3 eV and more structure in the E₁ series of transitions. These features show that the structural superlattice has an effect on the bandstructure. The shift of the E₀ level to lower energies can be explained by using a simple model based on the Kronig-Penney approximation.

The spectrum for the (4:4) structure is shown at the bottom of Figure 2. In this sample,

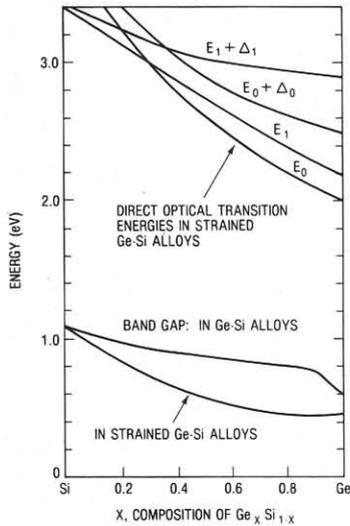


Figure 1: Bandgap transition energies for strained Ge-Si alloys grown on a (001) Si substrate. The Si substrate imposed a biaxial compressive strain on the Ge-Si layer that reached 4% when pure Ge is grown on Si.

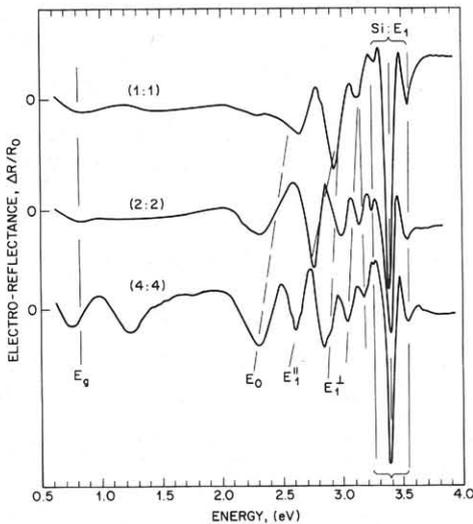


Figure 2: Electro-reflectance spectra for a (1:1), (2:2) and (4:4) atomic-layer superlattices grown on (001) Si. The spectrum for the (1:1) superlattice resembles that of a random alloy. The (2:2) and (4:4) spectra are more complex and demonstrate the effect of the superlattice on the energy band structure.

the complexity seen in the (2:2) structure is further developed. In addition, new optical transitions are seen at 0.8 and 1.2 eV. By comparing with Figure 1, it can be seen

that no direct optical transitions occur in this energy range for any Ge-Si alloy.^[5,6] The origin of these transitions can be explained in part by folding of the Brillouin zone by the superlattice potential.^[7] However, since the indirect bandgap for this material lies at lower energies (about 0.6 eV and 300K), these superlattices are all indirect bandgap materials.

Theoretical calculations have shown that indirect bandgap behavior is expected for all Ge-Si superlattices grown on Si (001) substrates.^[7-13] However, these same calculations hold out promise that some superlattices grown on (001) Ge substrates may have a bandgap that is more direct in character.

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