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The electronic structure of Si/Ge superlattices

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Abstract. We have calculated the electronic structure of Si/Ge superlattices grown on (111)-orientated substrates. The band offsets are determined from the local density of states.

Among the important parameters characterising a heterojunction are the band offsets. Model theories of band offsets define a reference level for each semiconductor which is then used to align the bulk band structures of the constituents. Van de Walle and Martin [1] were able to determine the band offsets by lining up the average potentials on

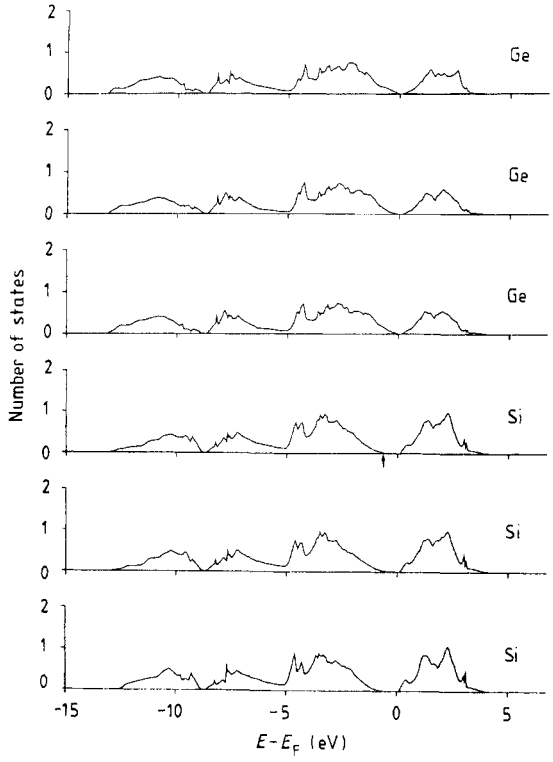

Figure 1. The LDOS across the $(Si)_6/(Ge)_6$ superlattice structure.

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either side of the interface. The average potentials were obtained from a self-consistent calculation of the interface structure. The method of matching average potentials is limited in that it does not take proper account of the interface detail. The local density of states (LDOS) has been used quite successfully to study the factors influencing the Schottky barrier heights at silicide/silicon interfaces [2].

Our calculations were performed on Si/Ge superlattices using standard norm-conserving non-local pseudopotentials in the local density approximation. The atom positions in these strained systems were obtained using a valence force-field model. Plane waves with kinetic energies up to 11 Ryd were considered. In figure 1 below we show the LDOS for the superlattice calculation. From the difference in the valence band maxima, we estimate the valence band offset to be 0.5 eV. This compares favourably with other calculations [1, 3] and experiment [4].

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