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Band offsets at InAs/GaAs interfaces

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Abstract. The electronic band structures of InAs/GaAs superlattices are calculated and band offsets determined from the local density of states.

The InAs/GaAs strained interface has attracted much attention in recent years due to its technological importance [1]. The valence band offsets are very much dependent on the atom positions and hence on the amount of strain. In this preliminary study, we

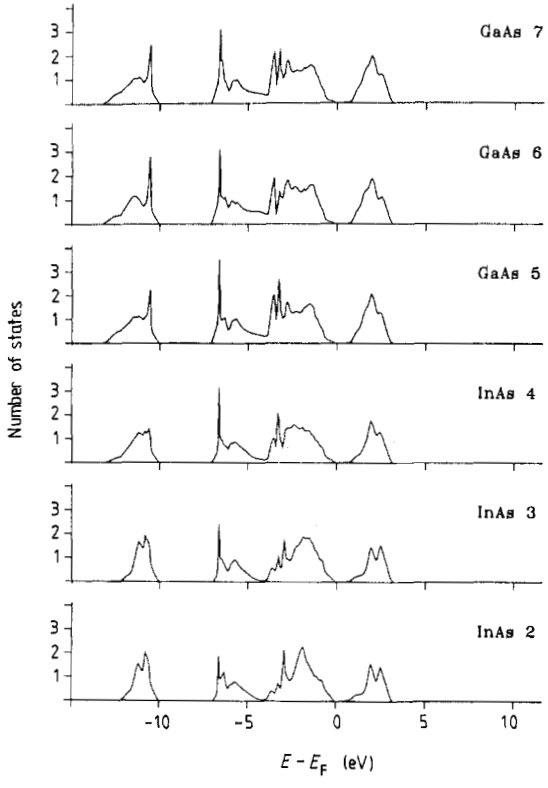

Figure 1. The LDOS across the InAs/GaAs superlattice structure. (In GaAs 7, InAs 4 etc the numbers are layer numbers.)

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report on calculations performed for InAs/GaAs superlattices on (100) $In_{0.5}Ga_{0.5}As$ substrates. Thus, in this instance, both semiconductors are strained. The atom positions were obtained using a valence force-field approach.

The self-consistent calculations were performed using standard non-local norm-conserving pseudopotentials with plane waves corresponding to an energy cut-off of 9.5 Ryd. The valence band offset is the difference between the valence band maxima and can be obtained directly from the local density of states across the superlattice. This technique has been used quite successfully to study silicide/silicon [2] and Si/Ge [3] interfaces. From figure 1, it can be seen that the difference between the maxima is very small. We estimate the value to be 0.06 ± 0.05 eV. Priester and co-workers [1] found the valence band offsets for InAs/GaAs to be 0.47 eV for GaAs substrates, -0.34 eV for InAs substrates, and 0.03 eV for InP substrates. This is in good agreement with our results, as the lattice spacing for InP is nearly equal to that of $In_{0.5}Ga_{0.5}As$. The results also agree well with experiment [4].

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