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LETTER TO THE EDITOR

A method for determining band offsets in semiconductor superlattices and interfaces

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Abstract. The long-standing problem of determining band offsets at semiconductor interfaces is readdressed and a new method for obtaining these values is proposed. *Ab initio* self-consistent pseudopotential calculations have been done on the Si/Ge and InAs/GaAs systems and the band offsets in specific cases determined. The problem of band offsets in superlattices is also investigated with particular reference to the superlattice period length and orientation. The existence of these band offsets is found to depend strongly on the localisation of some of the valence or conduction bands in either of the constituents.

In recent years there has been a lot of work done on determining bands offsets at heterojunctions from self-consistent interface calculations. Van de Walle and Martin (1987) performed first-principles calculations on a number of different interface structures and were able to determine the band offsets by first calculating the differences between the average total potentials, $\Delta \bar{V}_{av}$, of the two constituents. This together with the respective bulk band structures (taking strain into account where required) yielded the valence band offset, ΔE_v. Baldereschi *et al* (1988) used a similar approach for the GaAs/AlAs interface but considered the electrostatic potential across the interface rather than the total potential. Huang *et al* (1989) reported that ΔE_v for the Si/GaP heterojunction could be obtained directly from the interface band structure by identifying which valence band states had predominantly Si bulk properties and which had GaP properties. All these methods give band offsets in the correct range of experimental and model calculation values. In this paper we propose another way of obtaining the band offsets from a knowledge of the electron local density of states (LDOS) across the interface and the bulk density of states. This method has the added advantage of giving information on the extent of interface states, localisation of electrons and also the band offsets in superlattice structures and their dependence on the superlattice period. Louie and Cohen (1975) were the first to plot the LDOS across an interface structure and read off the valence band maxima. This approach will, however, only be possible in cases where either the interface states are very highly localised, or the superlattice period is large. The method we have used is similar to the one used by Rees and Matthai (1988) to estimate the Schottky barrier heights at silicide–silicon interfaces. The LDOS across the interface and also the DOS of the constituent bulk semiconductors (with strain included where appropriate) is calculated. The latter is then fitted to the LDOS of the 'bulk-like' layers. Since the reference scale is determined by the interface calculation, ΔE_v is simply the difference between the valence band maxima of the bulk DOS. Because

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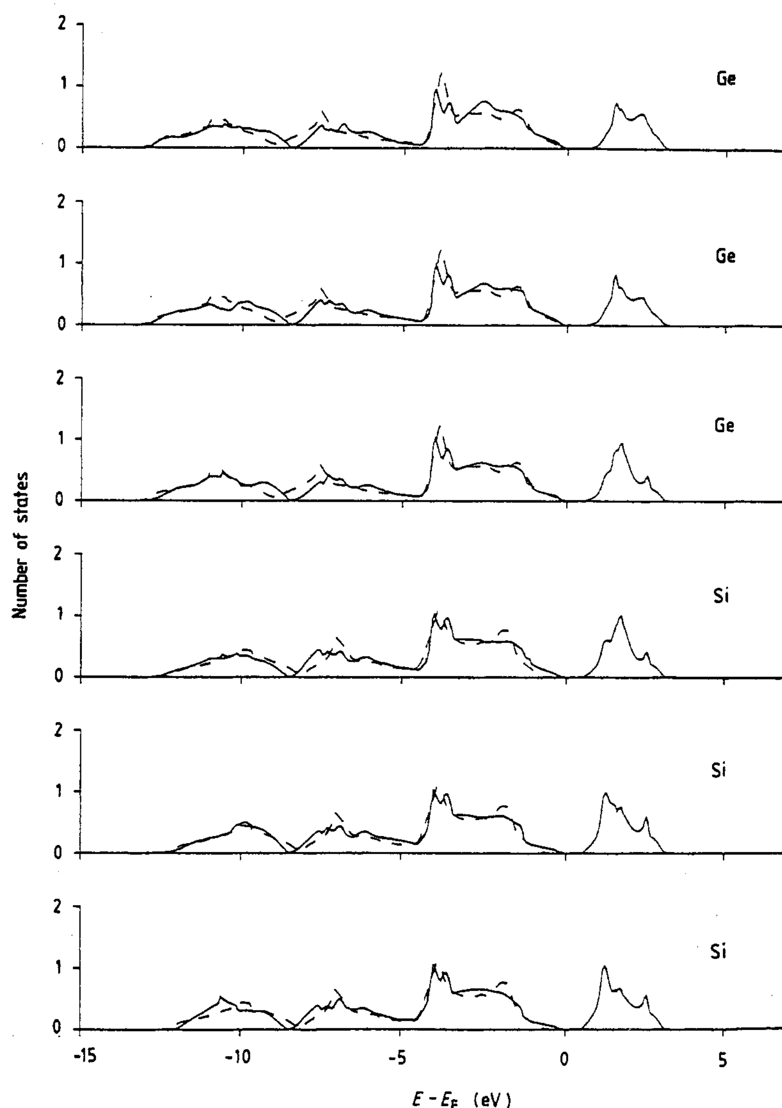

Figure 1. The LDOS (full curves) across half the $(Si)_6/(Ge)_6$ superlattice together with the bulk DOS of Si and strained Ge (broken curves).

of the presence of interface states, the fitting was done using a least squares method, so the main peaks in the bulk DOS are reproduced as closely as possible. As a test of this method we have also calculated $\Delta \bar{V}_{av}$ and the corresponding ΔE_v. Further, we present the results for two very different strained systems so as to establish the credibility of this approach.

The calculations were carried out using non-local, norm-conserving, *ab initio* pseudopotentials within the local density functional framework. Plane waves up to 11 Ryd were included and a special-point scheme was used to sample k-space. In figure 1, we show the LDOS for a (001) $(Si)_6/(Ge)_6$ superlattice strained on a Si substrate. The spin–orbit interaction was not included *a priori* into the calculation. The atomic coordinates

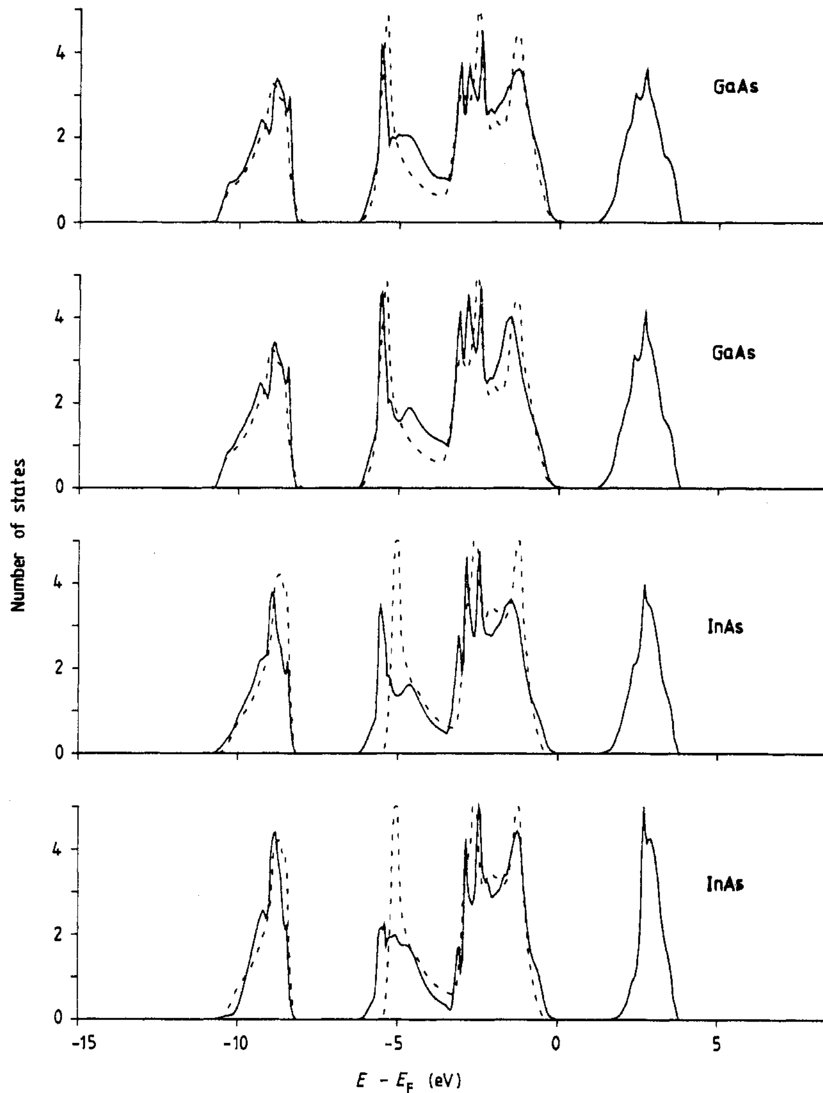

Figure 2. The LDOS (full curves) across half the $(GaAs)_3/(InAs)_3$ superlattice together with the bulk DOS of strained GaAs and InAs (broken curves).

were obtained using a Keating force field model with the parameters fitted to the *ab initio* total energy calculations of Froyen *et al* (1988). From LDOS results we find that $\Delta E_v = 0.65$ eV which is in good agreement with the value of 0.76 eV obtained using the average potential method.

In figure 2, we show the results for the (001) $(GaAs)_3/(InAs)_3$ superlattice strained on an InAs substrate. In this case, the fitting is not as good as for the Si/Ge system. However, it can be seen that the fit for the middle layers is better than for the interface layers showing the decay of the interface states. The valence band offset is estimated to be -0.67 eV compared with the -0.6 eV obtained with the average potential method. The reason for the small discrepancy between the DOS and the LDOS for the 'bulk-like'

layers is due to the relatively short period of the superlattice considered, and to the long range Coulomb interaction which is more important in this ionic system. When doing the fitting, it is important to use the same energy cut-offs and equivalent k-point meshes for both bulk and interface calculations.

In the superlattice band structure, strain effects lead to a splitting of the valence bands. In some special cases, some of the valence band states (or conduction band states) are highly localised. These states can be identified by plotting the average charge density associated with the states across the interface. When such localisation does occur, the superlattice structure itself displays a band offset as was shown for the (111) Si/Ge interface (Bass and Matthai 1989a, 1989b). The value of the offset is the calculated valence band splitting. When such localisation occurs, the particular bands can be identified with either of the superlattice constituents as was done by Huang *et al* (1989). However, it is important to stress that the band offset of the superlattice is not identical to that at the interface. For example, for the (111) $(Si)_n/(Ge)_n$ interface, the band offset for the $n = 6$ superlattice was found to be 0.53 eV compared with the value of 0.85 eV calculated for the interface. Also this superlattice band offset increases with increasing n. So for example, the states for (111) $(Si)_{12}/(Ge)_{12}$ are more localised and the valence band splitting also increases. In the limit as n becomes very large, the two results should become identical. Morrison *et al* (1987) in considering very long period Si/SiGe superlattices and using an empirical pseudopotential method showed that localisation does indeed occur for these structures, and that band offsets could thus be obtained. Another point to note is the dependence of the superlattice band offset on orientation. For the (100) $(Si)_n/(Ge)_n$ system, there is little or no localisation of electrons for the n = 6 superlattice structure. However, on increasing n, there is a trend towards increasing localisation and a widening of the valence band splitting. Within the limits of the calculation, the interface band offset appears to be independent of orientation.

The main conclusions that can be drawn from this study are that the band offsets at a semiconductor heterojunction interface can be obtained directly from a knowledge of the LDOS and that some semiconductor superlattices also exhibit band offsets. The latter depends on the period of the superlattice and on the orientation. In the limit of long periods, the superlattice and interface band offsets become identical.

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