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LETTER TO THE EDITOR

Tailoring materials for quantum wells: band offsets at (001)-oriented GaAs/$(AlAs)_n(GaAs)_m$ interfaces

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Abstract. The electronic structure at the interface between bulk GaAs(001) and short-period superlattices of $(AlAs)_n(GaAs)_m$ has been calculated using *ab initio* pseudopotential techniques. Our results show that the valence band offsets at such interfaces are very similar to those obtained experimentally for random alloy systems, but superior transport properties are anticipated for the ordered systems.

Short-period superlattices form a new kind of bulk material [1], whose electronic properties differ from other systems. Compared with random alloys [2] of the same nominal composition, the superlattices should, for instance, have significantly better transport properties. This makes them interesting in device applications, for example MODFET structures, lasers and photodetectors. High-quality epitaxial interfaces between different semiconductors can be grown by techniques such as molecular beam epitaxy (MBE) [3]. The most important parameters characterising such heterojunctions are the valence and conduction band offsets.

In this paper, we present first-principles calculations of band offsets for the heterojunctions (GaAs)(001)/$(AlAs)_n(GaAs)_m$, for $n = 1, 2, 3$; $m = 1$ and $n = m = 2$. Our calculations were performed using a supercell geometry, and were based on local-density-functional theory [4]. From the self-consistent potentials we obtained information about potential shifts at the interface, including charge rearrangement. Combining this with two bulk band-structure calculations allowed us to derive the band offsets. These offsets are compared with experimentally derived ones for interfaces involving random $Al_xGa_{1-x}As$ alloys.

The geometry used for the interface and for the short-period superlattices was an ideal zincblende structure ($a = 5.65$ Å), continued throughout the system without any displacements of the atoms from their ideal positions. In the (001) direction there is one kind of atom in each layer, and the interlayer separation is $0.25a$. The interface ($z = 0$ in figures 1 and 2) consists of one such layer of the common anion species. In the supercell calculation [5–9] the number of atoms in each unit cell was taken sufficiently large that the central parts on either side of the interface have bulk-like characteristics (charge densities, potentials etc). It was established *a posteriori* that this is the case. All calculations were performed within the framework of the local-density-functional theory

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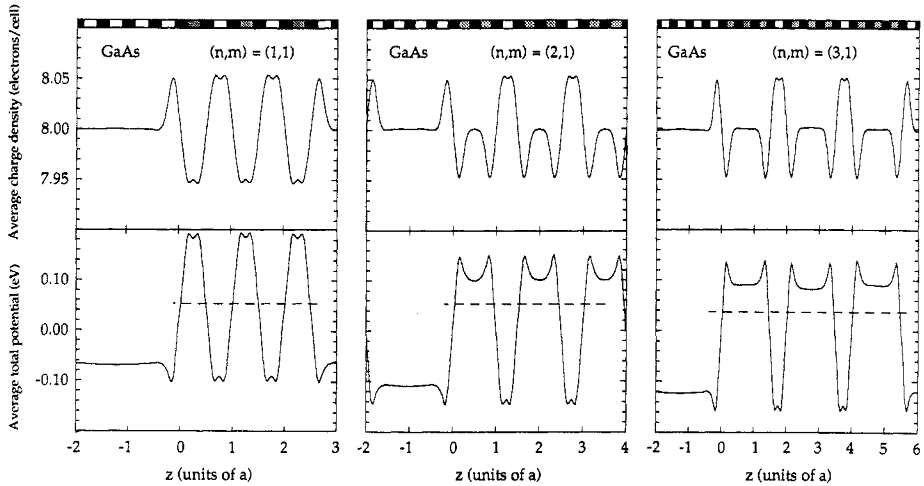

Figure 1. Average charge densities (top panel) and the corresponding average total potentials (bottom panel) for $(AlAs)_n(GaAs)_m$ superlattices on GaAs(001). The broken horizontal lines in the bottom panel represent the average total potential in bulk $(AlAs)_n(GaAs)_m$. The common As plane is at $z = 0$ (one atom/layer and interlayer distance $0.25a$). The As, Ga and Al atomic layers are schematically indicated by black, white and grey boxes respectively.

[4] applied in the momentum space formalism [10, 11] using non-local, norm-conserving, *ab initio*, pseudopotentials [12] and the Ceperley–Alder form of the local-density approximation for exchange and correlation [13]. The k-space integrations were performed using a special-points technique. We have used a (442) Monkhorst–Pack mesh [14] and plane-wave basis sets up to 10 Ryd kinetic energy, other than for the simple GaAs/AlAs interface, where a 14 Ryd cut-off was used. In the main calculations, in which interfaces between GaAs and various short-period superlattices were studied, the GaAs substrate was represented by eight layers and the superlattice structure was varied as shown in figure 1. Convergence studies with respect to the size of the basis set and the supercell have been performed for $(n, m) = (2, 1)$ and for the GaAs/AlAs interface, and indicate that the band offsets are converged to better than 0.05 eV for all systems.

The band offsets are extracted as follows. First a self-consistent supercell calculation is performed, and the charge density and total local potential thus obtained are averaged using a slab-averaging method [15]. Slab-averaged charge densities and total potentials for some interfaces are shown in figures 1 and 2. From bulk calculations for the two systems we obtain the valence band edges relative to the average total potential (see figure 3). The total potential includes the Hartree part, the local part of the ionic pseudopotential and the exchange–correlation part, i.e. the non-local part of the pseudopotential is not included in our reference potential. The spin–orbit interaction was not included in the density-functional calculations, which are scalar relativistic. These effects can be added in *a posteriori* by using experimental values for spin–orbit splittings, but these effects are relatively small, and we do not believe that their inclusion would have any bearing on the conclusions of this work.

To test our method of calculation we consider first the well known GaAs/AlAs interface (figure 2). The most recent data for the valence band offset range from 0.53 to 0.56 eV [16]. In our calculations, the band structure of each material is obtained relative

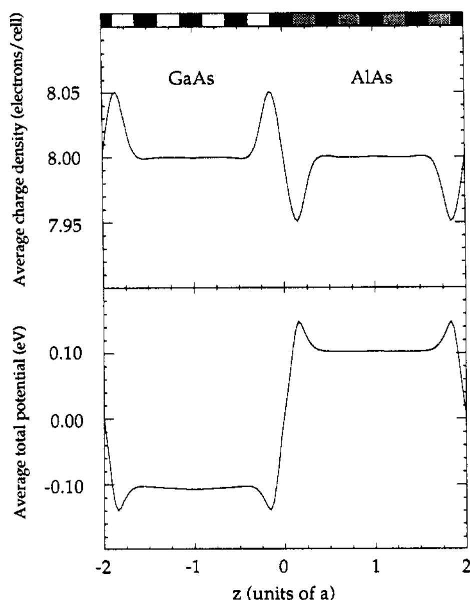

Figure 2. Average charge density (top panel) and the corresponding average total potential (bottom panel) for the simple GaAs/AlAs heterojunction. The common As plane is at $z = 0$ (one atom/layer and interlayer distance $0.25a$). The As, Ga and Al atomic layers are schematically indicated by black, white and grey boxes respectively.

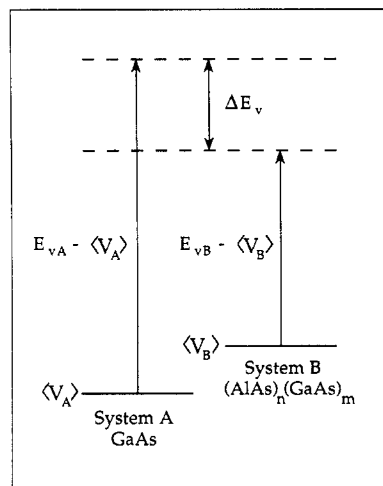

Figure 3. Derivation of band offset ΔE_v from the relative positions of the total average potentials (obtained from the supercell calculation) and the top of the valence bands relative to the total average potentials (obtained from two bulk calculations).

to the average of its own total potential (figure 3). Aligning these average potentials of GaAs and AlAs results in a difference between the valence band maxima of 0.61 eV. From addition of this quantity to the potential line-up (−0.21 eV; see figure 2(*a*)), we obtain 0.40 eV for the valence band offset. To compare with experiment we must take into account spin–orbit interaction and many-body corrections to the LDA result. The latter will increase the band offset by about 0.1 eV [17], while the effect of spin–orbit splitting will raise the band offset additionally by 0.02 eV [18]. Including these effects we obtain a theoretical value for the band offset of 0.52 eV, in good agreement with experiment.

We compare our results for the $(AlAs)_n(GaAs)_m$ interface with those for the corresponding interfaces between GaAs and *random* $Al_xGa_{1-x}As$ alloys. In these random alloys the band gap increases with x, and for $x \geqslant 0.43$ changes from direct to indirect. In contrast to the alloy system, the band gap in $(GaAs)_2/(AlAs)_2$ is direct [2].

In figure 4 the band offsets are shown as a function of the effective value of x, together with the experimental values for the corresponding alloys. For the $(n, m) = (2, 2)$ interface (not shown in the diagram) we obtain an offset of 0.22 eV. The short-period superlattice offsets show a similar trend to the alloy offsets [2] (the offset is $(0.5x)$ eV over the whole range $0 < x < 1$).

The quantites calculated are electronic ground state properties, while in principle the valence band edges are quasiparticle energies. Recent quasiparticle calculations using the GW approximation for the self-energy operator have shown that corrections

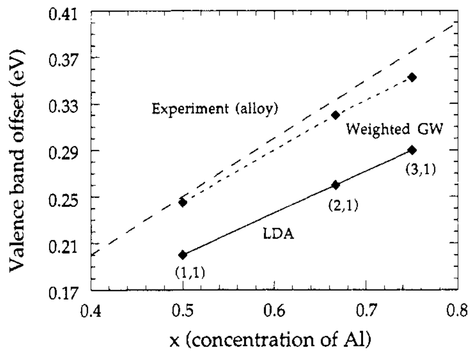

Figure 4. Calculated valence band offset for the ordered $(AlAs)_n(GaAs)_m$ system for different (n, m), compared with the corresponding random alloy.

to the local-density-approximation valence band maxima are similar for bulk GaAs (0.13 eV above the LDA valence band edge) and bulk AlAs (0.04 eV above the LDA valence band edge [17]. If we approximate the self-energy correction to the valence band edge in $(GaAs)_m(AlAs)_n$ by a weighted average of bulk GaAs and AlAs corrections, we obtain a band offset curve that is remarkably close to that for the alloy (figure 4).

As already mentioned, the alloy with $x = 0.5$ has an indirect band gap but the corresponding superlattices $(GaAs)_m(AlAs)_m$ with $m \geqslant 2$ have direct band gaps [2]. A practical advantage with the superlattice system would therefore be a higher mobility than the corresponding alloy, since at Γ the electron effective mass is relatively small. Furthermore, the electrons in all the superlattices are free from alloy scattering which should also give better transport properties.

In summary, we have calculated valence band offsets for short-period superlattices $(AlAs)_n(GaAs)_m$ on GaAs (001) using self-consistent supercell techniques. The valence band offsets are very similar to those of the corresponding alloy interfaces, (GaAs)/ $(Al_xGa_{1-x}As)$, but we expect superior transport properties for the ordered system.

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