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Electronic structure of InGaAs and band offsets in InGaAs/GaAs superlattices

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Abstract. We report the results of self-consistent density functional calculations using *ab initio* pseudo-potentials on $In_xGa_{1-x}As/GaAs$ superlattices for $x = 0.25, 0.5, 0.75$ and 1.0. The calculations were performed for two strained configurations. It was found that for GaAs substrates the valence band offset was almost independent of In content. For the case of $In_xGa_{1-x}As$ substrates, the valence band offset appears to vary non-linearly with the amount of strain in the GaAs layer. As a precursor to obtaining the band offsets, the electronic band structure of InGaAs was calculated for different compositions and strain conditions. These results are analysed and compared with experiment.

1. Introduction

There has been much interest in the study of the electronic properties of strained layer superlattices in recent years. The elastic strain gives an extra degree of freedom in the engineering of new device structures. The InGaAs/GaAs system has the further advantage in that the indium content x, can also be altered giving even more flexibility. Thus, the wide range of physical properties available in these strained superlattice structures allows for the construction of optimized materials for device applications.

For electronic devices, the values of the band discontinuities (ΔE_v, ΔE_c) across the heterojunction interfaces are important parameters. For the InGaAs/GaAs system, most published results usually report the ratio of the conduction band offset to the difference in the band gap, $Q_c = \Delta E_c/\Delta E_g$. There has been some controversy regarding the dependence of Q_c on the indium concentration with claims that it is independent of x [1] and counter claims that the results can be reinterpreted in a way that suggests a concentration dependence [2]. Also, a range of values has been reported for Q_c varying from 0.4 to 0.8 [3, 4]. For $x = 1$, i.e. InAs strained onto GaAs, Q_c was found to be 0.83 from x-ray photoelectron spectroscopy [5]. For thick layers of InAs on GaAs, which are strain relieved, transport measurements suggest a value for Q_c of 0.72 eV [6]. Thus, if Q_c is relatively independent of In concentration, it would be natural to suppose that Q_c has a value around 0.8. No calculations have been reported (to our knowledge) on this system for the whole range of values of x. Although the amount of strain is very large, with modern growth techniques, it is now possible to grow pseudomorphically strained short period InAs/GaAs superlattices. Hence, it is important to study the InGaAs/GaAs system for all values of indium composition.

In this paper we report on the results of calculations on the InGaAs/GaAs superlattice structure and, in particular, the dependence of the valence (and conduction) band

offset on strain and In compositions. Because the method used to extract these offsets demands knowledge of the electronic structure of the constituent semiconductors, we have also performed calculations on the $In_xGa_{1-x}As$ ternary alloy for different values of the composition parameter, x.

2. Calculation method

All the electronic structure calculations were performed in a supercell geometry using non-local norm-conserving pseudopotentials as described by Bachelet *et al* [7]. Spin–orbit splitting effects were included *a posteriori* in the manner described by Van de Walle [8].

The band offsets were determined by first calculating the self-consistent potential across the interface structure. This potential is then averaged in the two (A, B) constituent regions, away from the interfaces. The difference in these potential averages, $\Delta\bar{V} = \bar{V}_A - \bar{V}_B$, is the important parameter in determining the band offset. The electronic energies of the two bulk constituents are then calculated with respect to the average total potentials and these are aligned in such a way that the difference in the bulk average potentials was put equal to $\Delta\bar{V}$. The valence band offset is then simply the difference in the valence band maxima ($\Delta E_v = E_v^A - E_v^B$). Thus, calculations on the bulk systems (including strain where appropriate) as well as on the interface structure need to be performed. This approach is the same as the one used by us to investigate band offsets at the InAs/GaAs interface [9].

3. Electronic structure of $In_xGa_{1-x}As$

To obtain the band offset for the $In_xGa_{1-x}As$/GaAs system, it is necessary to have a knowledge of the band structure of the bulk $In_xGa_{1-x}As$ alloy. There have been both experimental and theoretical studies of this alloy system. Hwang *et al* [10] used angle resolved photoemission spectroscopy to study the band structures of GaAs and $In_{0.2}Ga_{0.8}As$ strained on GaAs as well as the unstrained $In_{0.2}Ga_{0.8}As$. A comparison of the band structures shows a shifting down of $\Delta_3 + \Delta_4$ (i.e. $(P_x + P_y)$-like) band along ΓX in strained $In_{0.2}Ga_{0.8}As$ by 0.15 eV and an upward shift of the Δ_1 (P_z-like) band by 0.25 eV. These shifts are opposite to that observed in strained GaAs. Stampfl *et al* [11] studied the $In_{0.27}Ga_{0.73}As$ alloy and obtained similar results. Boguslawski and Baldereschi [12] performed *ab initio*, self-consistent pseudopotential calculations on $In_xGa_{1-x}As$ ($x = 0.25, 0.5, 0.75$) and found that the large bowing of the band gap is a result of the repulsion between the lowest conduction bands and higher levels folded from the X-point of the Brillouin zone.

In the $In_xGa_{1-x}As$ ternary alloy, each As atom had four nearest neighbours which may be either In or Ga atoms. These four atoms make a basic tetrahedral unit and there are only five such units possible. The alloy unit cell is accordingly constructed from these types of basic units. We considered the $In_xGa_{1-x}As$ alloy with x taking values 0.25, 0.5, 0.75 in a tetragonal unit cell with four or eight atoms per cell.

Because of the unequal bond lengths (i.e. InAs and GaAs) present in the alloy system, it was necessary to determine first the atomic coordinates for the minimum energy configuration. This was done by using the Keating valence force field model to minimize the energy [9]. The resulting bond lengths for the various In compositions are shown in table 1.

Table 1. Variation of the InAs and Ga–As bond lengths (in Å) in the unstrained and biaxially strained alloy InGaAs as a function of the indium concentration, x.

	Unstrained		Strained	
x	Ga–As	In–As	Ga–As	In–As
0.00	2.448	—	2.448	—
0.25	2.463	2.592	2.448	2.580
0.50	2.475	2.603	2.444	2.578
0.75	2.488	2.610	2.441	2.576
1.00	—	2.623	—	2.575

For the electronic structure calculations, an energy cut-off of 12 Ryd was found sufficient to give energy eigenvalue convergence to within 0.1 eV. This corresponds to ~1000 and ~500 plane wave for the 4 atom cell^{-1} and 8 atom cell^{-1} cases. The band structures of the alloys show similar features to that of bulk InAs and GaAs. However, even accounting for the folded bands in the larger unit cell alloy systems, there are important points to note. At the top of the valence band at Γ, the degeneracy is broken even in the absence of spin–orbit or strain effects. It is directly due to the presence of unequal bond lengths in the unit cell. Also, at symmetry points the electron energies in the alloy are not simple averages of those found in InAs and GaAs. Furthermore, the energy separations vary with k-vector. It can therefore be concluded that the potentials in the alloy cannot be regarded as an average of the constituent potentials (virtual crystal approximation). As an illustration of these effects we show the band structure, in particular symmetry directions, of $In_{0.25}Ga_{0.75}As$ together with those of InAs and GaAs in figure 1. The band structure of the alloy is in general agreement with the experimental results of Stampfl *et al.* The computed band gaps have also been calculated and are displayed in figure 2. Experimentally, the band gap variation of the unstrained alloy is found to vary with indium concentration according to [13]

$$E_g = 1.5192 - 1.5837x + 0.475x^2 \text{ eV } (2\text{ K}).$$

The band gaps are, as expected, smaller than the experimental values because of the use of the LDA in our calculations. However, it should be noted that the LDA correction is neither constant nor does it vary linearly with the size of the band gap. Also, the band-gap variation clearly exhibits the bowing effect, i.e. the reduction of the band gap with respect to the linearly interpolated value between the GaAs and InAs bandgaps, although the bowing factor (>1) is larger than the experimental value. This shows once again, that the electronic properties of InGaAs cannot be considered as being linearly dependent on the composition. This non-linearity can easily be interpreted as due to the difference in the lattice constants of InAs and GaAs. Zunger and Jaffe [14] have shown that the band gap in the semiconductor alloys based on lattice mismatched compounds is reduced by internal lattice distortion. Mikkelsen and Boyce [15] arrived at similar conclusions after making bond length measurements in InGaAs using the extended x-ray adsorption fine structure technique. The bond lengths calculated by us (table 1) are in very good agreement with the experimental findings.

To investigate the effect of strain on the electronic properties of the alloy, we also performed calculations of InGaAs under biaxial strain, with the lattice constant reduced in two dimensions to that of GaAs. The equilibrium configuration was once again determined by energy minimization. The alloy band gap variation with x is displayed in

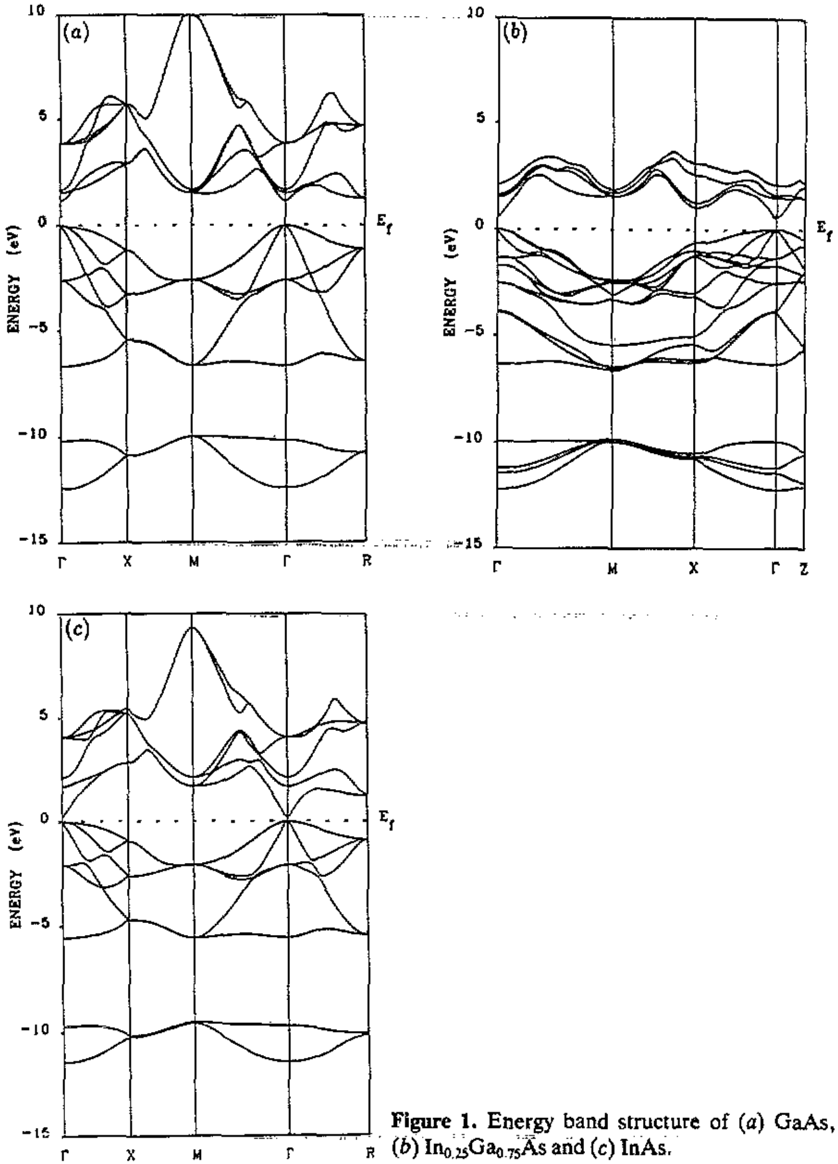

Figure 1. Energy band structure of (*a*) GaAs, (*b*) $In_{0.25}Ga_{0.75}As$ and (*c*) InAs.

figure 2. Strain has the effect of considerably reducing the bowing in the band gap variation. Although the bowing factor is different, the general trend of band gap variation is in accordance with the experimental results of Ji *et al* [4] which can be interpreted as giving the band gap dependence of $In_xGa_{1-x}As$ biaxially strained on GaAs as

$$E_g = 1.5192 - 1.1557x + 0.163x^2.$$

The effect of the strain on the band structure is found to be in agreement with experiment [10] and can be seen by comparing the band structure of strained $In_{0.25}Ga_{0.75}As$ (figure 3) with that of the unstrained alloy (figure 1) and figure 2 of [10]. Another quantity of importance in the study of band offsets at interfaces is the valence band splitting due to strain. In figure 4 is shown the valence band splitting for InGaAs strained on GaAs substrates. It can be seen that this variation is almost linear with composition.

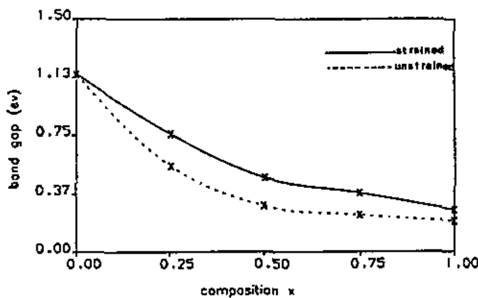

Figure 2. Energy band gap of unstrained (broken curve) and strained (full curve) of $In_xGa_{1-x}As$ as a function of composition.

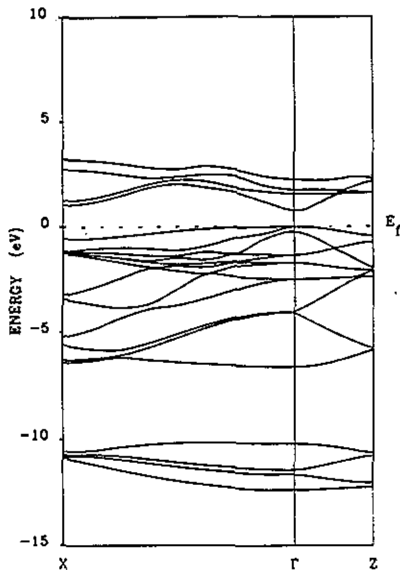

Figure 3. Energy band structure of $In_{0.25}Ga_{0.75}As$ strained on to a GaAs substrate.

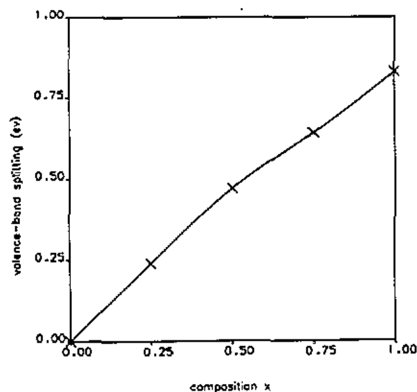

Figure 4. Variation of the valence band splitting in the $In_xGa_{1-x}As$ alloy strained on to a GaAs substrate as a function of composition.

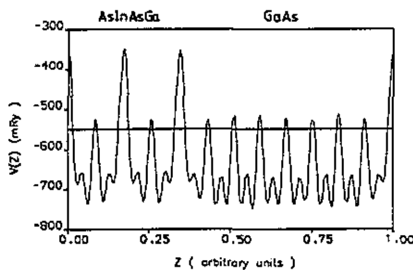

Figure 5. Averaged self-consistent potential $\bar{V}(z)$ across the InGaAs/GaAs [001] interface.

4. Band offsets at InGaAs/GaAs interfaces

As mentioned above, the band offset at a heterojunction arises from two contributions. The first is the difference in the average total potentials of the two constituent semiconductors and is called the potential line-up. The other contribution comes from the band edges with reference to the average potentials. The latter is affected by strain in that the band edges are shifted with respect to their original positions according to deformation potential theory. In the alloy the band edges are also affected by the composition. The potential line-up is dominated by the interface dipole which in turn has been shown to be critically dependent on strain, inter-atomic distances at the

Table 2. Valence band offset ΔE_v at the $In_xGa_{1-x}As$/GaAs interface for different substrate lattice constants, a_{SLC}. Also given are the differences in the average potentials, $\Delta \bar{V} = \bar{V}_{InGaAs} - \bar{V}_{GaAs}$, and the Q_c values for GaAs substrates.

a_{SLC} (Å)	x	$\Delta \bar{V}$ (eV)	ΔE_v (eV)	Q_c
5.653	0.00	0.00	0.00	—
5.653	0.25	0.33	0.02	0.95
5.653	0.50	0.66	0.05	0.93
5.653	0.75	0.99	0.07	0.92
5.653	1.00	1.32	0.09	0.92
5.759	0.25	0.32	−0.25	
5.865	0.50	0.62	−0.48	
5.962	0.75	0.87	−0.64	
6.058	1.00	1.16	−0.68	

interface [9] and the type of bonding at the interface [16]. It has also been shown that this dipole can be altered by the judicious introduction of layers of another material at the interface [17, 18].

To determine the potential line-up for the different alloy/GaAs interfaces, two sets of calculations were done, namely, for $In_xGa_{1-x}As$ strained on GaAs and for GaAs strained on $In_xGa_{1-x}As$. Once again alloys with $x = 0.25$, 0.5, 0.75 and 1.0 were considered. For $x = 0.25, 0.75$, the unit cell consisted of two layers each of GaAs and InGaAs making 20 atoms cell^{-1}, whereas for $x = 0.5$, the unit cell had 24 atoms which comprised of three layers of the alloy and six layers of GaAs. The atom positions were determined by minimizing the distortion energy using the VFF formalism. The purpose of these interface calculations was to determine the difference in the average potentials $\Delta \bar{V}$ in the two regions, and so it was necessary only to have self-consistency in the total potential. An energy cut-off of 6 Ryd was found sufficient to provide convergence in the planar average potential which goes to the bulk potential values one atomic layer from the interface.

The valence band offsets, determined by aligning the bulk band structures taking into account the average potential difference, $\Delta \bar{V}$, thus obtained are given in table 2. For GaAs substrates the valence band offset varies linearly. However, the small magnitude of ΔE_v implies a large value of Q_c which remains approximately constant. Thus, our results would appear to support the results of Anderson *et al* who find a high value of Q_c for indium concentrations up to $x = 0.4$. To understand why Q_c is constant, it is necessary to study the two contributions to ΔE_v in a little more detail. The increased strain in InGaAs for larger values of x alters the interface dipole and increases $\Delta \bar{V}$ linearly with x. There is also a linear increase in the magnitude of the valence band splitting (figure 4) with x which shifts the valence band edge with respect to the average position of the top three valence bands, $E_{v,av}$. However these shifts are compensated by the downward movement of $E_{v,av}$, due to the hydrostatic component of the biaxial strain. The net result is to keep ΔE_v close to zero with only a small rise with increasing x.

For InGaAs substrates, $\Delta \bar{V}$ still increases with x, but now it is a result of a lowering of the average potential of GaAs which is under increasing strain. This is not a linear increase as was found for InGaAs under compressive strain. The average position of the top three GaAs valence bands moves up in energy under the hydrostatic component of the biaxial strain and the uniaxial part causes a splitting of these states which further shifts the valence band edge with respect to the average potential. Thus, the consistent increase in $|\Delta E_v|$, with the GaAs valence band edge above that of InAs is almost wholly

due to the band edge movement. From table 2 is should be noted ΔE_v increases non-linearly with increasing x, for $x > 0.5$. This is due to the non-linearity in the behaviour of $\Delta \bar{V}$ with x as well as due to the electronic energies in InGaAs not being simple (linear) averages of those in InAs and GaAs.

5. Conclusion

From the results of our calculations, we conclude that for $In_xGa_{1-x}As$ grown on GaAs, the conduction band offset ratio, Q_c, is constant with a value of about 0.9. For GaAs grown on $In_xGa_{1-x}As$, the valence band offset increases with x but in a non-linear way. We have also calculated the band structure of $In_xGa_{1-x}As$ for different values of x and have shown that for $x = 0.25$, the results for both unstrained and strained layers, are in good agreement with the experimental work done on samples with $x = 0.20$ and $x = 0.27$.

The work was intended as a study of the variation of the band offset in heterojunctions as a function of strain and composition. The results are in contrast with those found for the Si/Ge_xSi_{1-x} heterojunction [19], where it was found that the valence band offsets depended linearly on both the alloy composition x and on the substrate lattice constant.

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