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Band offsets in strained layer superlattices

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Abstract
Band offsets at semiconductor heterojunctions have been shown to be critically dependent on a number of factors. By applying the ab-initio pseudopotential method to the strained InGaAs/GaAs superlattice, we have been able to determine the dependence of the offsets on the strain in the system and on the indium composition. In addition, we have shown that it is possible to control the interface band discontinuities by the introduction of an interlayer of Ge at the interface.

Keywords: lattice- mismatched, strained layer

1. Introduction

Semiconductor - semiconductor interfaces or heterojunctions of lattice mismatched systems like In GaAs / GaAs have attracted much attention in recent years due to the flexibility in tailoring band-gaps and for possible applications in high-speed optoelectronics devices [1]. In these systems strain as well as composition can be used to vary the barriers to electrical transport across the heterojunction. These band offsets are among the most important parameters which determine the optoelectronic properties and so it is of outmost importance to have a knowledge of how they vary with strain and composition. Although model theories have enjoyed some success in predicting the band offsets at different heterojunctions, they are not able to account for the influence of the details of the interface structure. To do this, self-consistent interface calculations which can correctly describe the charge transfer across the interface must be performed.

Recent theoretical investigations on the influence of strain on the band offsets of InAs/GaAs suggest that these quantities are markedly dependent on strain [2]. However, because of the large lattice-mismatch for this system, the critical thickness before the onset of strain relief is less than four atomic layers. As a result, there are no reliable experimental data for the strained InAs/GaAs system. In contrast, the In_xGa_{1-x} As/GaAs system has been the subject of much study especially for the low values of the x [3]. However, even for this system there has been some controversy as to whether the ratio of the conduction band offset to the difference in the band-gaps, $Q_c = \frac{\Delta E_c}{\Delta E_g}$, is independent of the indium content [3]. In addition to the dependence of the band offsets on the electronic structure of the bulk constituent semiconductors, the interface dipole also plays an important role in determining the band lineup. In many applications involving heterojunctions, the ability to control or tune the barriers to electrical transport for a given pair of semiconductors is highly desirable. Recently, it has been shown that it is possible to alter the band offsets by changing the interface dipole through the introduction of dopant layers confined to a very narrow region in space(δ - doping) either at or near to the interface[4].

We have undertaken a systematic study of the InGaAs/GaAs system with a view to obtaining a quantitative understanding of how the band lineups vary with the strain in the system, the indium composition and the interface dipole. Strain was varied by considering the interface structure to be constructed on different substrate lattices. The dipole was altered by the

introduction of a double layer of Ge at the interface. Before we describe the results of these calculations, we first outline the calculational procedure and indicate how the band offsets were determined from the self-consisternt calculations.

2. Calculation procedure

The calculations were performed in a supercell geometry using the pseudopotential method within the Local Density Approximation (LDA) with the Hedin-Lundqvist [5] representation for the exchange-correlation potential. Because of the need to correctly describe the charge transfer across the interface, norm-conserving, non-local pseudopotential [6] were employed. It is well known that the use of the LDA results in incorrect conduction band energies. This will undoubtedly affect the band lineups. However, if it is assumed that LDA corrections are very similar for both InAs and GaAs, the effect on the band offsets would only be second order in comparision with strain and dipole effects.

The band offsets can only be obtained directly from the interface calculation if the supercell used is sufficiently large to mimic a true interface. As this would involve an inordinately large number of atoms, the discontinuities were obtained by a two-step process. Initially, the band structures of GaAs and InGaAs strained onto a substrate of known lattice constant were calculated, each with respect to a reference level. This level was taken to be the average of the total potential seen by the electrons, $\bar{V}$. The interface calculations were then performed so as to align the two reference levels, $\bar{V}$ (InAs) and $\bar{V}$ (GaAs).

Because, in these calculations it is only necessary to obtain self- consistency in the difference of the average potentials, $\Delta\bar{V}$, fewer plane waves are sufficient than would be required for self- consistency in the electronic energies. Once the reference levels are properly aligned, the valence band offset is simply the difference in the valence band maxima, $\Delta E_v = E_v$ (InAs)- E_v (gaAs). The conduction band offset can then be determined from a knowledge of the band gaps, $\Delta E_c = \Delta E_g - \Delta E_v$.

For the calculations of the bulk electronic energy bands it was found that the plane waves up to an energy of 12 Ryd were sufficient to provide eigenvalue convergence to within 0.01 eV. To simulate the strained bulk materials, tetragonal unit cells with four or eight atoms were used with the atomic positions being determined by minimising the total energy. The interface structures were modelled by a supercell with up to 24 atomic layers and a Keating valence force field model [7] was used to establish the equilibrium positions of the atoms. Plane waves with energies less than 6 Ryd were used in these calculations.

Once self- consistency in the total potentials, $V(r)$ was achievied, it was averaged in the planes parallel to the interface. The $\bar{V}(z)$ across the interface displays a discontinuity as it moves from the bulk-like InAs region to the bulk-like GaAs region. The average potentials in the two bulk regions were then determined, and the resulting $\Delta\bar{V}$ used to align the bluk energy bands.

3. Results

a. Strain

To investigate the effect of strain without any other complications, calculations were performed on InAs/GaAs superlattices ranging from that of bulk GaAs(5.65Å) to that of bulk InAs(6.08Å). The effect of strain on the band discontinuities manifests itself in two ways. The biaxial strain can be separated in to hydrostatic and uniaxial contributions, both of which cause a shift in the position of the valence band maximum. The conduction band minimum is only affected by the hydrostatic component. The magnitude of the shifts are given in terms of the standard deformation potential [8]. In addition to this, the average potential also undergoes a shift due to a change in the local atomic volume.

Because the band gaps of the strained materials are also altered, the conduction band offset will vary differently from that of the valence band offset. From the results of our calculations, we find that for InAs/GaAs strained on $In_yGa_{1-y}As$ substrate, the valence band offset can be reasonably represented by the equation:

$$\Delta E_v = 0.09\text{-}0.77y \text{ (eV)} \quad (1)$$

The conduction band offset can deduced from a knowledge of the band gap variation with y.

b. Composition

The effects of composition were investigated by performing calculation of $In_xGa_{1-x}As$ strained on a GaAs substrate and of GaAs strained on $In_xGa_{1-x}As$ substrates. For the calculations to be feasible, we only considered x = 0.25,0.50 and 0.75.

The calculational procedure was the same as for the InAs/GaAs system [2], except in this instance, the electronic structure of strained and unstrained InGaAs had also to be determined. For GaAs substrates, the valence band offset remains almost constant as the shift in the valence band maximum in the InAs is nearly cancelled by an opposite shift in the position of the average potential. The band discontinuities were found to approximately satisfy the equations:

$$\Delta E_v = 0.09x \text{ (eV)} \quad (2)$$
$$\Delta E_c = 0.92\Delta E_g \text{ (eV)} \quad (3)$$

where ΔE_g is the difference in the band gaps. The relative constancy in the Q_c value is in general agreement with experimental data [3].

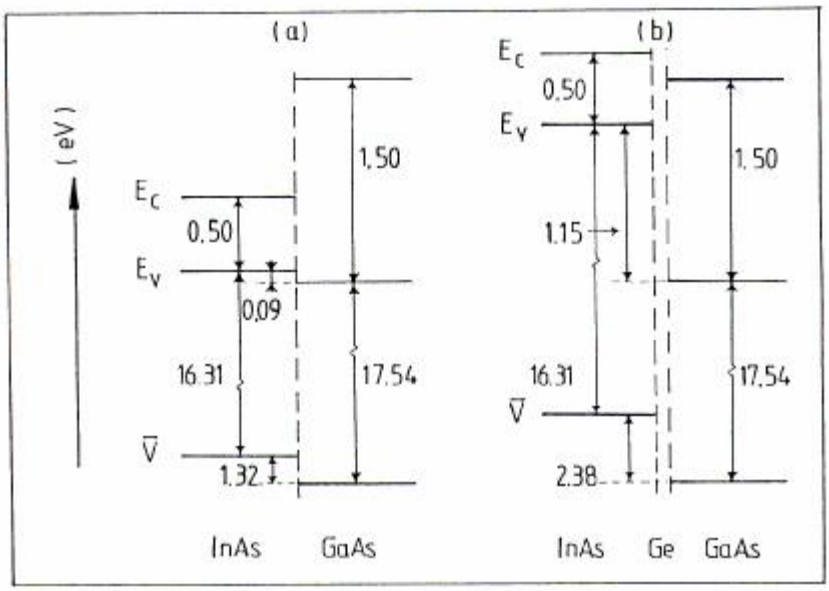

Figure 1. Schematic diagram of the band lineup in the :(a) InAs/GaAs and (b) InAs/Ge_2/GaAs interfaces.

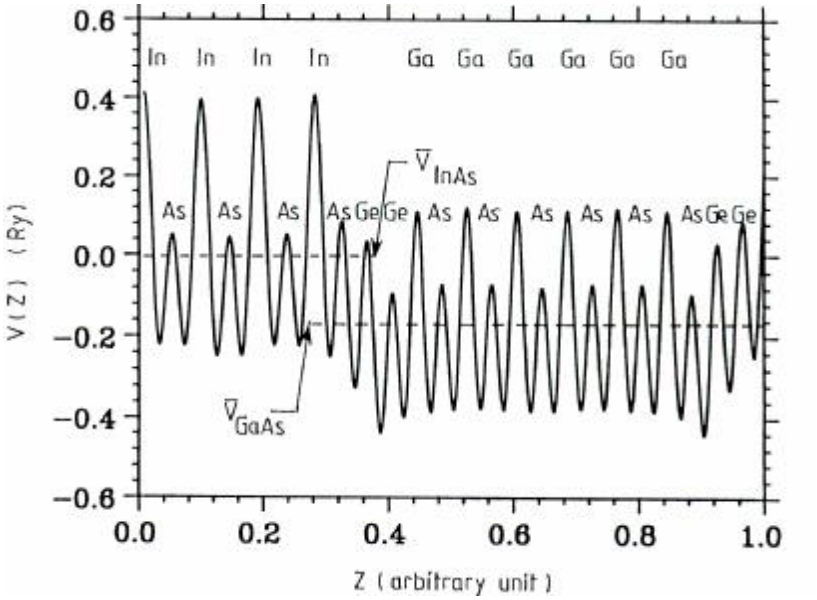

Figure 2. Averaged self-consistent potential $\bar{V}(z)$ across the [001] interface. The horizontal dashed lines show the potential averages, $\bar{V}_{InAs}$, $\bar{V}_{GaAs}$.

For InGaAs substrates, the GaAs is under tensile stress and so the shift in its valence band maximum adds onto the shift in the average potential resulting in the valence band offset varing non- linearly with the indium content

$$\Delta E_v \approx -x + 0.3\, x^2 \text{ (eV)} \qquad (4)$$

c. Interface dipole

As mentioned above the dipole at the intreface is critical in lining up the electron bands at the heterojunction. Interlayers of Ge were introduced at the two interfaces of the supercell. To simplify the calculation, two InAs layers were removed and replaced by two bilayers of Ge. As the number of electrons in the supercell remained unchanged, it was possible to still use the special points scheme to sample k-space. It should be noted that, experimentally, a δ-layer could consist of regions where the dopant is only a monolayer thick, and others where it is two or more layers thick. Hence, it is important to make a study of all the possible interface structures to

see which has the greatest impact on the band discontinuity. The results presented in this paper thus forms only the first part of a program to investigate the control of band offsets by δ-doping.

Two calculations were performed on supercells with 24 atoms comprising of 4 InAs layers, 6 GaAs layers and 4 Ge layers. In the first, the Ge layers were introduced in such a way that both interfaces were identical with the Ge bilayer lying between the In and As layers. Furthermore, the interface dipoles were in opposing directions resulting in zero field across the supercell. From the average potentials in the bulk-like regions, we found that the valence band offset increased from 0.09 eV for no interlayer to 1.15eV with the bilayer (Figures 1,2).This dramatic change in the band lineup can be attributed to the lack of charge flow from the Ge to In and As to Ge compared to the flow from As to In when no interlayer exists. In the second calculation, one Ge bilayer was placed between an As and an In layer as in the first case, but the other bilayer was placed between Ga and As layers. In this case there are two inequivalent interfaces with different dipoles, now in the same direction, resulting in a net field across the supercell. The band offsets at the interfaces are also different, with the valence band discontinuity at the As-Ge-Ge-Ga interface being modified to -0.6eV. Thus, we have shown that the direction and magnitude of the dipole are both important parameters in the control of the electrical barriers to transport.

4. Discussion

It should be borne in mind that the purpose of these calculations was not to predict accurate band offsets for a number of different interface configurations. Even if this were possible, it is very likely that such configurations could be realised experimentally. However these calculations provide information on the importance of the various factors in determining the band lineups and consequently can be used as a guide in the engineering of heterojunctions with particular properties. In performing all the calculations described above, we have found that the band offsets were critically dependent on the actual atomic positions at the interface. This would lead to uncertainties of ±0.1 eV in all the values reported. However, this would not invalidate any of the conclusions arrived at on basis of the calculations.

The major result of this work has been to show that although strain and composition have great influence on the band discontinuities at heterojunctions, the introduction of suitable layers modifying the interface dipoles affords the best way to engineer these barriers for specific device applications. The choice of the interlayer and its position is crucial and in fact allows for greater flexibility in tuning the band offsets.

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