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The nature of the Si impurity in ultrathin AlAs/GaAs superlattices

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Abstract. The electronic properties of n-type and p-type lightly doped $(AlAs)_n/(GaAs)_n$ ($n = 1, 3$) superlattices are investigated through a theoretical study using the calculation of the total, local and partial density of states by the recursion method in the tight-binding approximation. The influence of an impurity located in the bulk, at or near the interface, and on the surface of these systems has been studied. For all cases, the electronic structures of a substitutional Si atom is qualitatively more similar to that of a group-III atom than to a group-V atom. The shift of the bottom of the conduction band and the top of the valence band with different types of doping is discussed. We also report that there is a local field when a Si atom is located at the interface, which is different for n-type and p-type doping structures, and an electronic centre when Si is in the bulk. Furthermore, this paper indicates dehybridisation of the surface impurity.

1. Introduction

The electronic properties of substitutional impurities in AlAs/GaAs superlattices have recently been studied in some detail, and the binding energies of electrons and holes bound at such donors and acceptors, respectively, have been established by various studies [1–9]. These studies of the shallow impurity states in quantum wells (QWs) were initiated with the work in [1] in 1981. In that calculation, the problem of shallow impurity states in the simplest existing superlattices, i.e. states which can be considered as a set of independent QWs, were treated. Others [2, 3] have made realistic calculations for donor ground states and low-lying excited states using a finite-well barrier. In contrast with the above papers, in [4] the same problem in thin superlattices was discussed, taking into account the coupling of adjacent QWs. A general variational method developed in [5] was used in extensive calculations in [6–8] of the binding energy variations with well thickness, impurity position, etc. Recently in [9] the variational method was used to calculate the acceptor binding energies in AlAs/GaAs QWs with and without the application of electric, magnetic and uniaxial stress fields.

Previous theoretical work on impurities in superlattices has concentrated on the calculations of the donor or acceptor binding energies. As is known, the charge distribution of the electrons in a crystal is a characteristic function of many physical properties. In other words, most properties of solids including the binding energy, photoemission spectra and magnetism can be related to the density of states (DOS). What is the effect

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of impurities on the electron structure of a pure AlAs/GaAs superlattice? What kind of distribution of the valence electrons occurs around the impurity site? Are they localised or not? Therefore, it is a matter of common interest to study the DOS of an impurity and to investigate its influence on the electron structure of the pure AlAs/GaAs superlattices. The aim of this paper is to resolve these problems.

In general, the DOS is calculated from band-structure calculations (see, e.g. [10–12]). Very recently [13], Si donor states in heavily doped thin AlAs/GaAs superlattices were discussed using the self-consistent pseudopotential method, within the local-density formalism. It was shown that

(i) the donor impurity band is located about 0.1 eV below the bottom of the conduction band (CB) and

(ii) there is a slight tendency for the donor charge density to shift towards the GaAs region if the impurity is placed in the interface region.

However, the problem of the acceptor states and the case of an impurity placed on the surface were not treated. Also the model used was still the periodic ordered structure.

The general doping concentration in a semiconductor, and also in a semiconductor superlattice, is about 10^{15}–10^{18} cm^{-3} [14]. Therefore, it is clear that we could hardly use the heavily doped model in the discussion of impurity states of a superlattice in most cases. However, because the impurities break the periodic symmetry, the general band-structure calculation becomes difficult and even intractable.

In this work, we first investigate the electronic properties of a shallow Si impurity located in the bulk, at and near the interface, and on the surface of ultrathin AlAs/GaAs [001] superlattices, based on the tight-binding approximation, using the recursion method [15]. In contradiction to the model in [13], we do not use periodic conditions in our calculation. Because of the relatively small amounts of impurities used in n- or p-type doping superlattices, the distributions of these impurities in the structures is arbitrary. Also, we substitute a Si atom not only for a group-III atom, as done in [13], but also for a group-V atom. We believe that the model used here is more realistic. We shall see that the lightly doped AlAs/GaAs superlattices do give some very interesting results. In particular, we shall see small changes at the bottom of the conduction band (CB) and the top of the valence band (VB) due to different doping types. Similarly, small changes in the charge distribution of the electrons in the superlattices lead to an electronic centre in the bulk and to a local field at the interface around the impurity.

In § 2, we present a brief review of the method and models used to find the total DOS (TDOS), the local DOS (LDOS) and the partial DOS (PDOS) for each site in the doped (AlAs/GaAs) superlattices. In § 3, selected results are presented. On the basis of these models we shall discuss the electronic properties of the materials. Finally, in § 4, we summarise our results.

2. Model and method

Let us consider the structure of the [001]-oriented $(AlAs)_3/(GaAs)_3$ superlattices shown in figure 1. The atoms Al322 and As311 are located in the AlAs region, and the atoms of Ga978 and As965 in the GaAs region. The atom As966 is placed just at the interface, and Al323 and Ga976 are near the interface from the two sides, respectively. The number for an atom is how we label the atom in our calculated atom cluster. We discuss cases when a Si atom is substituted for a group-III atom or a group-V atom. In the same

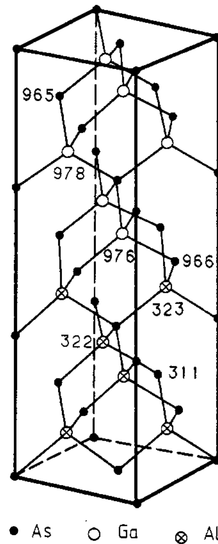

Figure 1. A pure $(AlAs)_3/(GaAs)_3$ superlattice cell.

way, we establish the calculated models for $(AlAs)_1/(GaAs)_1$ superlattices. Furthermore, the DOS of a (001) surface impurity and its influence on the electronic structure of neighbouring atoms in the $(AlAs)_1/(GaAs)_1$ system are also calculated.

The approach used in this paper is a first-principles method for calculating the electronic structure. It was developed in [15] within the tight-binding formalism. Because the method does not depend on long-range periodicity, it is especially useful for discussing the local environment around a defect and for giving the LDOS on each site in crystals. We choose the Hamiltonian matrix in the LCAO representation. Its elements are Slater–Koster integrals, i.e. the linear combinations of transition integrals between orbitals which were obtained in [16]. Only nearest-neighbour interactions between atoms are considered.

The atom cluster including $5 \times 5 \times 5$ crystal cells for $(AlAs)_1/(GaAs)_1$ structure and $5 \times 5 \times 2$ crystal cells for the $(AlAs)_3/(GaAs)_3$ structure is used for calculating each model. The recurrence chain length is selected as $L = 30$. We have calculated some models with a recurrence chain length $L = 50$ and find the results are almost the same as those obtained with $L = 30$. This has also been confirmed by us in other papers [17, 18].

By integration of the TDOS we can determine the Fermi energy in each case; this is -0.5238 Ryd for an $(AlAs)_1/(GaAs)_1$ and -0.6534 Ryd for an $(AlAs)_3/(GaAs)_3$ superlattice. We find that the Fermi energy decreases with increase in the number of monolayers per slab.

3. The electronic properties of Si-doped AlAs/GaAs superlattices

3.1. The changes in the bulk electronic structure

The influence of impurity Si on the bulk electronic structure of $(AlAs)_3/(GaAs)_3$ can be illustrated by calculation of the TDOS, LDOS and PDOS functions (figures 2–6). Only some of the projected DOSs are shown. The results in figures 2(*d*), 2(*h*), 3(*d*) and 3(*h*) for pure $(AlAs)_3/(GaAs)_3$ serve as 'reference'. First we consider the case formed by

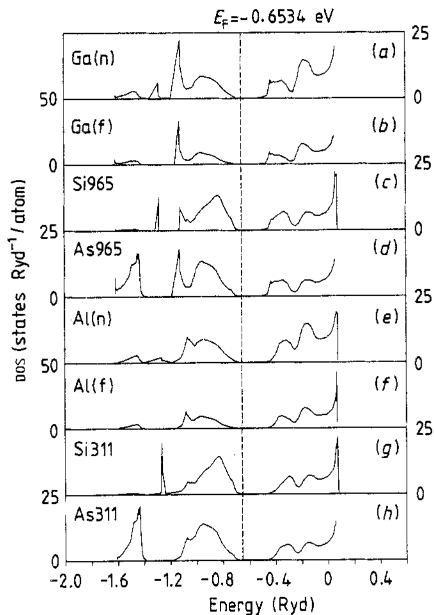

Figure 2. LDOSs of an impurity and its neighbouring atoms when a Si Atom is substituted for an As atom in the bulk. The notations n and f represent the atom near to and far from the Si atom, respectively.

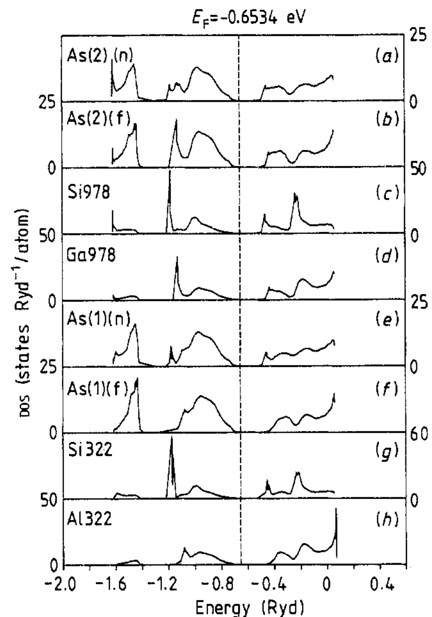

Figure 3. LDOSs of an impurity and its neighbouring atoms when a Si atom is substituted for a group-III atom in the bulk (As(1) is in the AlAs region; As(2) is in the GaAs region).

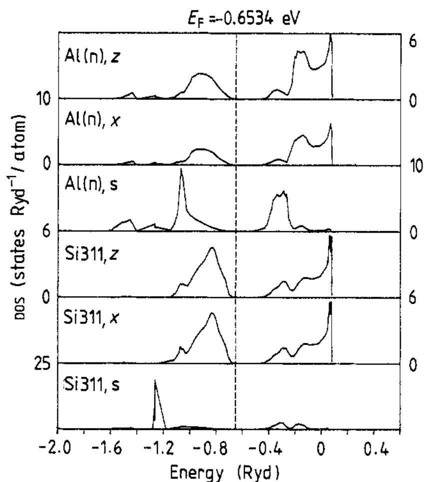

Figure 4. PDOSs of a Si atom and its neighbouring Al(n) atom in the AlAs region.

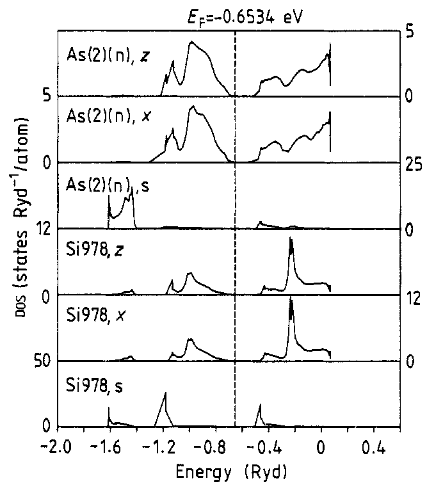

Figure 5. PDOSs of a Si atom and its neighbouring As(n) atom in the GaAs region.

replacing the As311 atom by the Si311 atom in the AlAs layer (figure 2(*g*)). The Al(n) atom (figure 2(*e*)) near to the impurity has essentially the same shape and magnitude as the Al(f) (figure 2(*f*)) far from the impurity. However, it is easy to see that there will be some states in the gap (from -1.20 to -1.40 Ryd) of the VB in a pure $(AlAs)_3/(GaAs)_3$ superlattice when it is doped with Si. This is because the peak of the Si s states shifts about 0.2 Ryd towards E_F compared with that of As s states. This increases the interactions

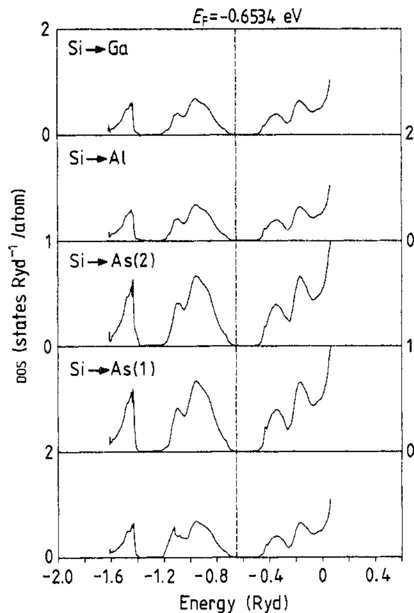

Figure 6. TDOSs of a crystal cell for different models. Si → As(1) and Si → As(2) represent a Si atom which substitutes for an As atom in the AlAs and in the GaAs region respectively.

between Si s states and Al(n) s and p states, which can be seen in figure 4. The influence of impurities on the electronic structures of $(AlAs)_3/(GaAs)_3$ due to substitution of Si965 for As965 in the GaAs layer has similarities with the above model (see figures 2(*a*)–2(*c*)).

The DOS in doped $(AlAs)_3/(GaAs)_3$ superlattices where a Si atom is substituted for a Ga or an Al atom, is given in figures 3 and 5. Comparing between figures 2(*g*) and 2(*h*) or between figures 3(*g*) and 3(*h*) (or between figures 2(*c*) and 2(*d*) or between figures 3(*c*) and 3(*d*)), we find that the shapes of the DOSs of a doping Si atom is qualitatively more similar to that of a group-III atom than to an As atom, but the amplitudes are larger. This reflects the fact that the doping Si is more likely to lose a p electron and then forms three sp^3 bonds with the neighbouring As atoms.

The calculated energy gap is about 0.16 Ryd for $(AlAs)_1/(GaAs)_1$ and 0.14 Ryd for $(AlAs)_3/(GaAs)_3$; these values are in concordance with the results given in [19]. We prove that the energy gap in $(AlAs)_n/(GaAs)_n$ decreases with increasing number of monolayers per slab. This has been testified by recent experiments [20].

Figure 6 shows the TDOS in doped and undoped $(AlAs)_3/(GaAs)_3$. As is known, the top of the VB is derived from the As anion p states, and the bottom of the CB from the Ga or Al cation. The work in [21] on thin superlattices of GaAs/AlAs indicates that the lowest unoccupied state is localised in the AlAs region. In the n-type doping case, the shift of the CB bottom with respect to the bottom of the pure $(AlAs)_3/(GaAs)_3$ CB is about 0.01 eV. This fact reflects the character of the shallow impurity in our problem. The Si-related impurity band in heavily doped thin AlAs/GaAs superlattices is located about 0.1 eV below the bottom of the CB [13]. In the same way, we also obtain the shift in the top of the VB to be about 0.03 eV for p-type doped AlAs/GaAs superlattices.

3.2. Local field in the interface region

In [13] the impurity charge densities near the interface of heavily doped superlattices were reported. However, in the calculation, only the case when a Si atom is substituted

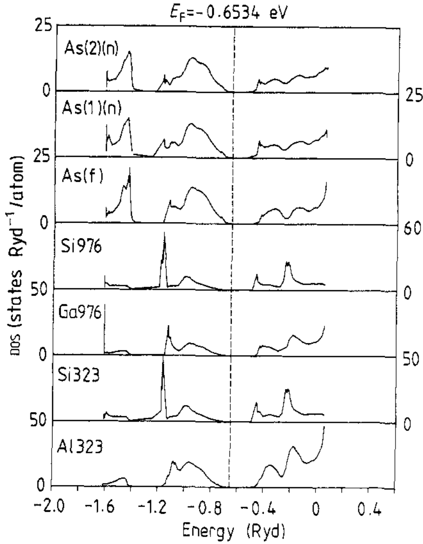

Figure 7. LDOSs of the atoms in the interface region when a Si atom is substituted for a group-III atom located near to this interface. As(1) and As(2) represent the interface As atom as a Si atom substitute for a neighbouring Al and Ga, respectively.

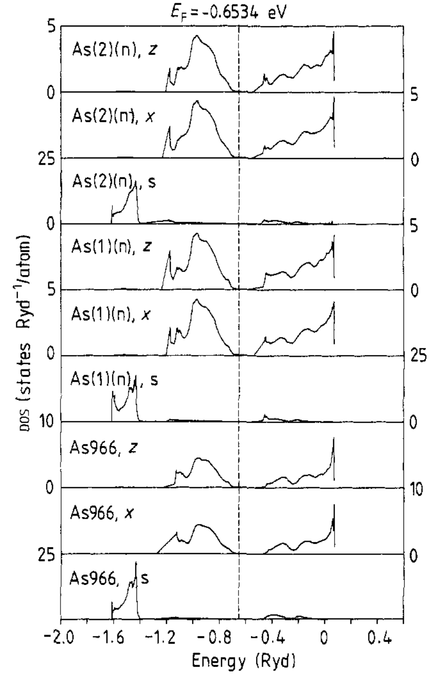

Figure 8. PDOSs of the interface As atoms given in figure 7.

for a Ga or an Al atom was considered. From the discussion in [13], we know that there is a local field set up around the Si impurity. Does this local field still exist in lightly doped superlattices? What will happen when we replace an interface As atom by a Si atom?

The DOSs of the Si atom and its neighbouring atoms are calculated for all three structures as Si → As, Si → Ga and Si → Al in the interface region. In our models, the interface is the As(001) plane which is perpendicular to the z direction. Figures 7 and 8 give the calculated results when a near-interface Ga or Al atom is replaced by a Si atom. Because of the influence of Si, the LDOS (corresponding to the CB) of the interface As atom is moved towards E_F. The slight change in the bottom of the host CB is about 0.01 eV for Si doping both in the AlAs layer and in the GaAs layer.

The valence electron number n_l that one atom possesses is determined by integrating its electronic DOS up to the Fermi energy. So the valence of an atom, which is apparently related to the energy distribution, can be given by the following equation:

$$\Delta N_l = N_l - n_l = N_l - \frac{1}{N} \sum_{\alpha, E_n \leqslant E_F} |\varphi^{\alpha}_{n(l)}|^2 \tag{1}$$

where N_l is the number of valence electrons on the free atom l, and $\varphi^{\alpha}_{n(l)}$ is the component of the eigenfunction corresponding to the valence orbital α on this atom.

We have given the valence of an atom in the interface region in table 1. From this table, it is easy to see that there is a local field set up around the impurity when a group-III atom is replaced by a Si atom and the direction of this field is towards the AlAs region. The reason for it is that the Al–As bond is more ionic relative to the Ga–As

Table 1. The valence of an atom in the interface region.

Atom	Valence	Atom	Valence	Atom	Valence	Atom	Valence
Al323[a]	0.1348	Si323	0.4229	As(n)[b]	0.0781	As(n)[c]	0.0225
Ga976[a]	0.0114	Si976	0.4273	As(n)[d]	0.1044	As(n)[b]	0.0514
As966[a]	−0.0698	Si966	−0.5007	Ga(n)	0.1059	Al(n)	0.0169

[a] These results are obtained from a pure $(AlAs)_3/(GaAs)_3$ structure which serves as a 'reference'.
[b] At the interface.
[c] In the AlAs layer.
[d] In the GaAs layer.

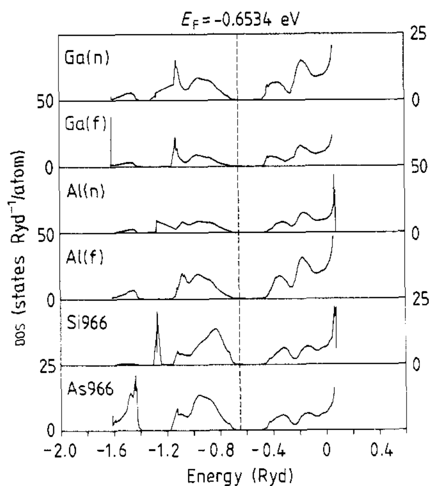

Figure 9. LDOSs of the atoms in the interface region when a Si atom is substituted for an interface As atom.

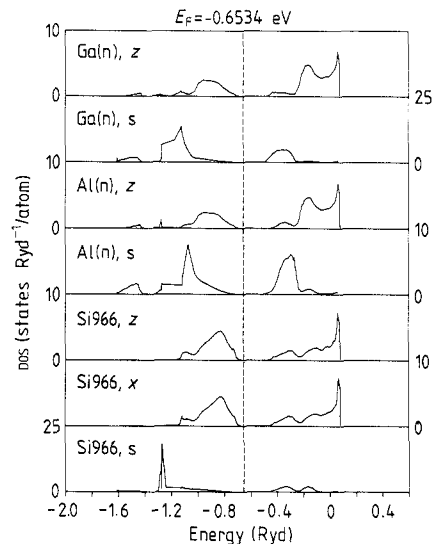

Figure 10. PDOSs of the atoms given in figure 9.

bond. Here we have precisely explained the shift of the impurity charge density into the GaAs region, which appears in figure 9 of [13].

Let us now return to the second question posed above, namely what will happen when an interface As atom is replaced by a Si atom? The LDOS and PDOS of the interface impurity Si and its neighbouring atoms are given in figures 9 and 10 respectively. In order to discuss the problem in more detail, we also calculated the valence of the corresponding atoms listed in table 1. We find a similar local field in the interface region, but note that its direction is towards the GaAs layer. It clearly shows the different influences of an impurity on the electronic properties of ultrathin AlAs/GaAs superlattices when we substitute a Si atom for a group-V atom or a group-III atom. This suggests that a small amount of impurity charge transfer towards the AlAs region occurs at the interface in p-type doped $(AlAs)_3/(GaAs)_3$ superlattices.

3.3. Electronic centre around the impurity Si

Using equation (1), all valences of the sites calculated are listed in table 2. Each site's

Table 2. The valence of an atom in the bulk of doped and undoped $(AlAs)_3/(GaAs)_3$.

	Pure structure				Doping structure			
Position	Atom	Valence	Atom	Valence	Atom	Valence	Atom	Valence
In AlAs region	As311	−0.1259	Si311	−0.5684	Al(n)	0.0127	Al(f)	0.1309
In AlAs region	Al322	0.1310	Si322	0.4190	As(n)	0.0224	As(f)	−0.1260
In GaAs region	As965	−0.0146	Si965	−0.4340	Ga(n)	−0.1027	Ga(f)	0.0121
In GaAs region	Ga978	0.0122	Si978	0.4310	As(n)	0.1044	As(f)	−0.0147

valence in this table is its average valence, e.g. the valence of As311 is −0.126, which means that As311 has possibilities of zero and minus one valence and so on. It is remarkable that the largest possibility of Al, Ga and As in pure $(AlAs)_3/(GaAs)_3$ superlattices is zero valence. Our results clearly show covalent interaction between a group-III atom and a group-V atom. Also, although our basic picture of the bonding in the system suggests sp^3 covalent bonding, the bonding is less complete or 'weaker' in AlAs than in GaAs.

It is interesting to note that the average valence of Si311 is −0.568 when we replace an As atom by a Si atom in the AlAs region. This is indicative of the largest possibility Si^- at the impurity site. We believe that there exists a negative electronic centre in the system. The reason for this is that the anion site has an atomic configuration $4s^24p^3$; this is the necessary atomic configuration to form the sp^3 bond with a group-III atom Al or Ga. When a Si atom, with atomic configuration $3s^23p^2$, is substituted at the anion site, it needs an extra p electron. In order to form the stable sp^3 bonds, it is possible for Si to trap an extra electron from other places. Consequently, there is hole conduction in p-type doped AlAs/GaAs superlattices. We have discussed the influence of Si on the neighbouring atoms. Our results show that the electronic structures of third-neighbour atoms are almost unaffected by the impurity. This confirms the fact that the charge density is localised around the Si impurity in the bulk case. The similar structure can be obtained if we substitute Si for As in the GaAs region. However, as we see in table 2, the possibility that Si traps an electron is lower in the GaAs region than in the AlAs region.

There is a positive electronic centre around the impurity when a Si atom is substituted for a group-III Ga or Al atom in the structure $(AlAs)_3/(GaAs)_3$. We can understand its character from the following argument. In this case the Si atom possesses an extra p electron which forms the sp^3 bond with the neighbouring As atoms. Consquently, the extra donor electron can occupy the non-bonding p state. It should be noted that the occupied non-bonding p state is contributed not only by Si p states but also by As p states; this is illustrated by our results listed in table 2. We have also proved that the main influence of Si is still in the third-neighbour atoms.

Furthermore, we show in table 3 the number of electrons in every orbital of Si under the Fermi level. It is notable that each s and p state in the Si atom may have about one electron when it is substituted for a group-III atom. This is in agreement with our earlier comments, which suggest sp^3 covalent bonding between Si and As (see also figure 8). When an As atom is replaced by a Si atom, there are more than about 1.5 electrons in the s state and one electron in each p state of Si. It is indicative of the basic picture of the covalent bonding in the system (figure 10).

Table 3. Numbers of electrons in partial waves of Si below the Fermi level.

Atom to be replaced by Si	Impurity	Number of electrons			
		s	p_x	p_y	p_z
Al	Si322	1.3671	0.7380	0.7380	0.7379
Al	Si323	1.3668	0.7368	0.7368	0.7367
Ga	Si976	1.3662	0.7355	0.7355	0.7355
Ga	Si978	1.3660	0.7343	0.7343	0.7344
As	Si311	1.5301	1.0129	1.0128	1.0126
As	Si965	1.5156	0.9728	0.9727	0.9729
As	Si966	1.5230	0.9927	0.9927	0.9923

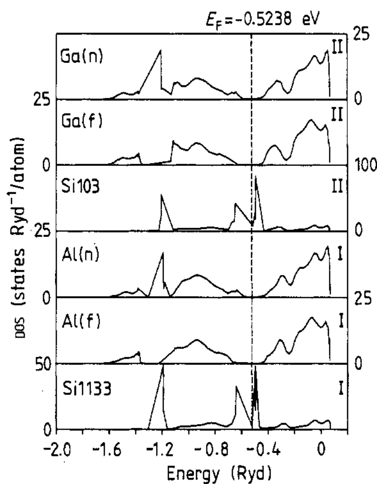

Figure 11. LDOSs of the surface atoms in models I and II.

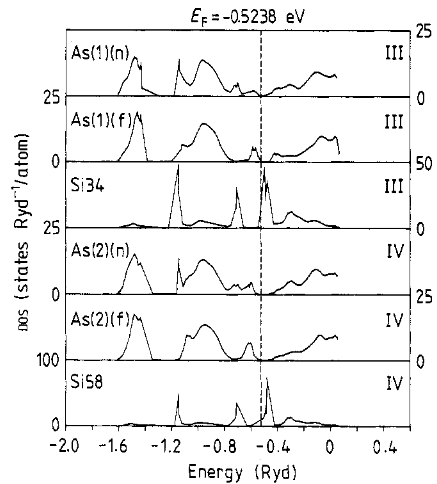

Figure 12. LDOSs of the surface atoms in models III and IV.

3.4. Dehybridisation at the surface

Because of the different bonding picture for the surface atoms and for the bulk and interface atoms, this will lead to a redistribution of the charge density. So it would be interesting to know the electronic structure of the surface impurity and its influence on the neighbouring atoms. We have calculated the electronic structure of Si localised at the (001) surface of the $(AlAs)_1/(GaAs)_1$ superlattice (figures 11–13). For convenience, the bulk Fermi level E_F is given in these figures.

In this section, according to the sequence of atom layers from the (001) surface we discuss four models:

model I: the As layer is the surface layer, and then the Al layer;
model II: the As layer is the surface layer, and then the Ga layer;
model III: the Al layer is the surface layer, and then the As layer;
model IV: the Ga layer is the surface layer, and then the As layer.

Figure 11 shows the LDOSs of the impurity Si when it is substituted for a surface atom As in models I and II. It is clear that there are some states in the band gap of the pure

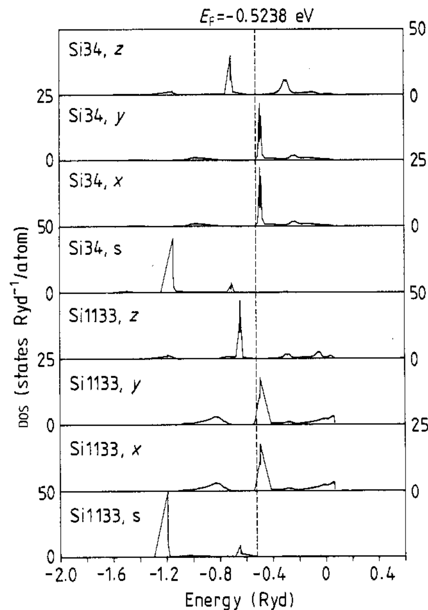

Figure 13. PDOSs of the surface Si atoms in models I and III.

$(AlAs)_1/(GaAs)_1$ structure which will make the bulk band edge bend at the surface. The results obtained from models III and IV are given in figure 12. We can see that the LDOS of As(n) corresponding to the CB shifts towards E_F. Thus the DOS has a value near E_F. The impurity DOS across the bulk Fermi level is mainly contributed by p_x and p_y states on Si. On the basis of these results, at least we can say that the effect of the surface impurity on the electronic structure of AlAs/GaAs superlattices should not be neglected when analysing experiments.

To identify the nature and origin of the various surface states, it is most helpful to consider the PDOS of a Si atom on the (001) surface (figure 13). Since the two broken sp^3 hybrid bonds are localised at the same atom, they interact very strongly, giving rise to pronounced dehybridisation, and consequently their symmetry character is entirely changed. Figure 13 shows clearly that there are a sp_z mixed dangling bond, which is oriented perpendicular to the surface, and a p_x–p_y mixed bridge bond, oriented along the [$\bar{1}$10] direction. The results agree well with all available experimental and theoretical reports [22–24]. From the energy viewpoint, we believe that surface reconstruction exists.

4. Conclusions

The electronic properties of n- or p-type doped AlAs/GaAs superlattices were discussed within the tight-binding approximation. The TDOSs, LDOSs and PDOSs in the bulk, in the interface region and on the surface of these systems have been calculated using the first-principles method. The results clearly show the local environment around an impurity. We have given the Fermi energies for $(AlAs)_n/(GaAs)_n$ (n = 1, 3) structures and determined the valence of each atom in doped $(AlAs)_3/(GaAs)_3$ superlattices. Furthermore, we obtained the number of electrons for every orbital of the Si atom under the Fermi level and show the influence of an impurity on its neighbouring atoms.

Our major results can be summarised as follows.

(i) The Fermi energy of ultrathin $(AlAs)_n/(GaAs)_n$ superlattices decreases with increase in the number of monolayers per slab.

(ii) The electronic structure of a substitutional Si atom is qualitatively more similar to that of a group-III atom than to a group-V atom.

(iii) The slightly smaller change in the bottom of the CB in the n-type, lightly doped $(AlAs)_3/(GaAs)_3$ system is about 0.01 eV, and the larger change in the top of the VB in the p-type doped system is about 0.03 eV.

(iv) There is a different local field around the impurity in the interface region in n-type and in p-type doped structures, which induces the shift of the charge density into the GaAs region in the former case and into the AlAs region in the latter case.

(v) An electronic centre is set up around the impurity in the bulk case.

(vi) The PDOS of a Si atom on the (001) surface shows that there are a sp_z mixed dangling bond and a p_x–p_y mixed bridge bond. This is indicative of the surface de-hybridisation.

(vii) In all cases, the charge density is highly localised around the shallow Si impurity.

Acknowledgments

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