

The interface charge transfer and internal electric fields in common-anion and non-common-ion superlattices

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1993 J. Phys.: Condens. Matter 5 7343

(<http://iopscience.iop.org/0953-8984/5/40/009>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.96

The article was downloaded on 11/05/2010 at 01:56

Please note that [terms and conditions apply](#).

The interface charge transfer and internal electric fields in common-anion and non-common-ion superlattices

Ren-Zhi Wang^{††}, San-Huang Ke^{††} and Mei-Chun Huang^{††}

[†] China Center of Advanced Science and Technology (World Laboratory), PO Box 8730, Beijing 100080, People's Republic of China

^{††} Department of Physics, Xiamen University, Xiamen 361005, People's Republic of China

Received 6 April 1993

Abstract. The hetero-interface of the common-anion superlattice (SL) $(\text{GaAs})_3(\text{AlAs})_3(001)$ is on the As atomic plane, while that of the non-common-ion SL $(\text{AlAs})_3(\text{GeGe})_3(001)$ is between the two atomic planes of As and Ge or of Ge and Al. In this paper, the self-consistent electronic structure calculation is reported for the two structures. The frozen-shape approach is used to determine the average bond energy and the valence band maximum in each molecular layer of the SL, and to investigate the relation between the interface structure and the internal electrical field. The results show that a large internal electric field exists in the non-common-ion SL but does not in the common-anion SL.

1. Introduction

It has been shown that the internal electric field in superlattices (SLs) is closely related to the orientation of the interfaces. Harrison *et al* [1] have shown that the internal electric field does not exist in Ge/GaAs(110) but does exist in Ge/GaAs(001). This electric field may be reduced or eliminated by the interdiffusion of different atoms at the interface. Eppenga's [2] work has also shown that, in the SLs constituted of two non-common-ion materials, namely ZnSe/GaAs, GaAs/Ge and ZnSe/Ge, an internal electric field exists in the (001)-oriented case, but does not in the (110)-oriented case. The present work shows that the internal electric field depends not only on the interface orientation but also on the interface structure. In this paper, using the linearized muffin-tin orbitals (LMTO) method within the atomic sphere approximation (ASA), the self-consistent band-structure calculations are reported for two different SLs: the common-anion SL $(\text{GaAs})_3(\text{AlAs})_3(001)$ in which the hetero-interface is on the As atomic plane, and the non-common-anion SL $(\text{AlAs})_3(\text{GeGe})_3(001)$ in which the hetero-interface is between two different atomic planes, i.e. between the As and Ge planes, or between the Ge and As planes. The average bond energy E_m and valence band maximum E_v in each molecular layer of SLs are investigated using the frozen-shape approach. By studying the relationship between the internal electric field, the interface structure and the charge transfer of valence electrons, the reason why the internal electric field exists in the non-common-ion SL but does not in the common-anion SL is analysed. In the next section the details of the calculation and the results are given. In section 3 the results are discussed.

2. Calculation method and results

2.1. The internal summation approach in the LMTO ASA method

The muffin-tin basis set adopted in the LMTO ASA band-structure method is

$$\chi_L^k(\mathbf{r}) = \frac{\Phi_{ilm}(-l-1, \mathbf{r}-\mathbf{q})}{\sqrt{S_l/2}\Phi_H(-)}\delta_{q'q} - \sum_{l'm'} \frac{\Phi_{l'l'm'}(l', \mathbf{r}-\mathbf{q})}{2(2l'+1)\sqrt{S_{l'}/2}\Phi_{l'l'}(+)} S_{L'L}^k \quad (1)$$

The corresponding secular matrix $\langle L'|H-E|L \rangle$ is given by the Ω and Π matrices:

$$H - E\mathbf{O} = \Pi[\Omega - (E - E\gamma)\Pi]. \quad (2)$$

Here

$$\Omega = [\omega(-)/\sqrt{S/2}\Phi(-)]_l \delta_{L'L} + \{\sqrt{S/2}\Phi(-)\omega(+)/[\omega(+)-\omega(-)]\}_{l'} S_{L'L}^k \quad (3)$$

$$\Pi = [1/\sqrt{S/2}\Phi(-)]_l \delta_{L'L} + \{\sqrt{S/2}\Phi(-)/[\omega(+)-\omega(-)]\}_{l'} S_{L'L}^k. \quad (4)$$

In equations (1)–(4), $L = t, l, m$, $S_{L'L}^k$ is the structure constant, and $\Phi(-)$, $\Phi(+)$, $\omega(-)$ and $\omega(+)$ are the potential parameters [3]. In the normal LMTO method, the L and L' generally consist of s, p and d states centred at each atomic site (the d state usually has a higher energy and is unoccupied; this is referred to as the ‘empty d state’ hereafter). In the ‘internal summation approach’ used in this paper, the L which determines the number of bases χ_L^k include only s and p states, while the summation index L' in equation (1) includes s, p and d states. That is the ‘empty d state’ is taken into account in the bases by the ‘internal summation’ of the tails of the muffin-tin orbitals. This is similar to using the Löwdin perturbation method to treat the ‘empty d state’ in order to reduce the size of the secular equation [4]. It has been shown that the valence band structure given by this approach is consistent with that given by the normal LMTO method [5]. This approach also gives reasonable results for the SL (GaAs)₁(AlAs)₁(001) [6] and bulk material MgO; in particular the results for MgO are very similar to those given by the *ab initio* pseudopotential method [7]. This approach is used throughout this paper.

2.2. Calculation of interface charge transfer and average bond energy

The lattice constants of AlAs, GaAs and Ge are nearly equal: 5.655 Å, 5.653 Å and 5.658 Å, respectively. So the SLs (GaAs)₃(AlAs)₃(001) and (AlAs)₃(GeGe)₃(001) can be considered to be lattice matched. The lattice constants of the SLs were taken to be $a = 5.654$ Å for (GaAs)₃(AlAs)₃(001) and (AlAs)₃(GeGe)₃(001). Because the above bulk materials and SLs belong to the tetrahedral structure (open structure), it is necessary to introduce ‘empty spheres’ into their unit cell for LMTO ASA calculations. For a bulk material AB (or CD), the primitive vectors of its unit cell are $\frac{1}{4}a(2, 2, 0)$, $\frac{1}{4}a(0, 2, 2)$ and $\frac{1}{4}a(2, 0, 2)$. Each unit cell contains two atomic spheres (A,B or C,D) and two empty spheres, which are located at $\frac{1}{4}a(0, 0, 0)$, $\frac{1}{4}a(1, 1, 1)$ and $\frac{1}{4}a(2, 2, 2)$, $\frac{1}{4}a(3, 3, 3)$, respectively. The SL (AB)₃(CD)₃(001) is a tetragonal structure; the primitive vectors of its unit cell are taken to be $\frac{1}{4}a(2, 2, 0)$, $\frac{1}{4}a(-2, 2, 0)$ and $\frac{1}{4}a(0, 0, 3)$. Each unit cell contains 12 atomic spheres and 12 empty spheres and can be divided into 12 atomic planes (or atomic layers). Two adjacent atomic layers constitute a molecular layer. All these are listed in table 1. In this paper, we assume that the volume of empty spheres is equal to that of atomic spheres. Ten special k -points

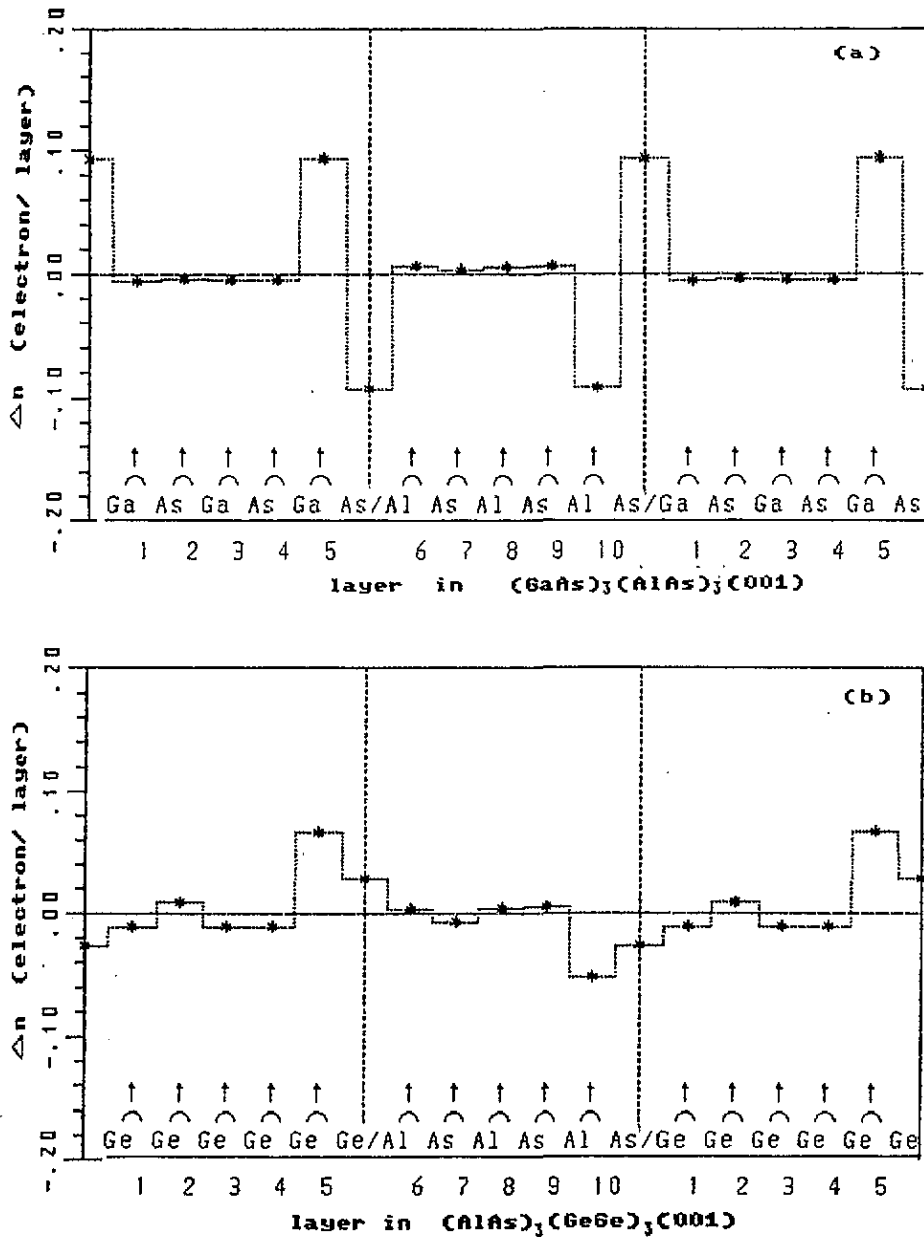


Figure 1. The distribution of excessive charge in SLs: (a) $(\text{GaAs})_3(\text{AlAs})_3(001)$; (b) $(\text{AlAs})_3(\text{GeGe})_3(001)$.

[8] are used for the self-consistent band-structure calculation of bulk materials and three special k -points [9] are used for those of SLs.

The valence electron number of each atomic sphere given by the band-structure calculations of bulk materials AB, CD and the constituted superlattice $(\text{AB})_3(\text{CD})_3(001)$ are listed in table 1. The valence electron charge contained in the three atomic layers (Ga,

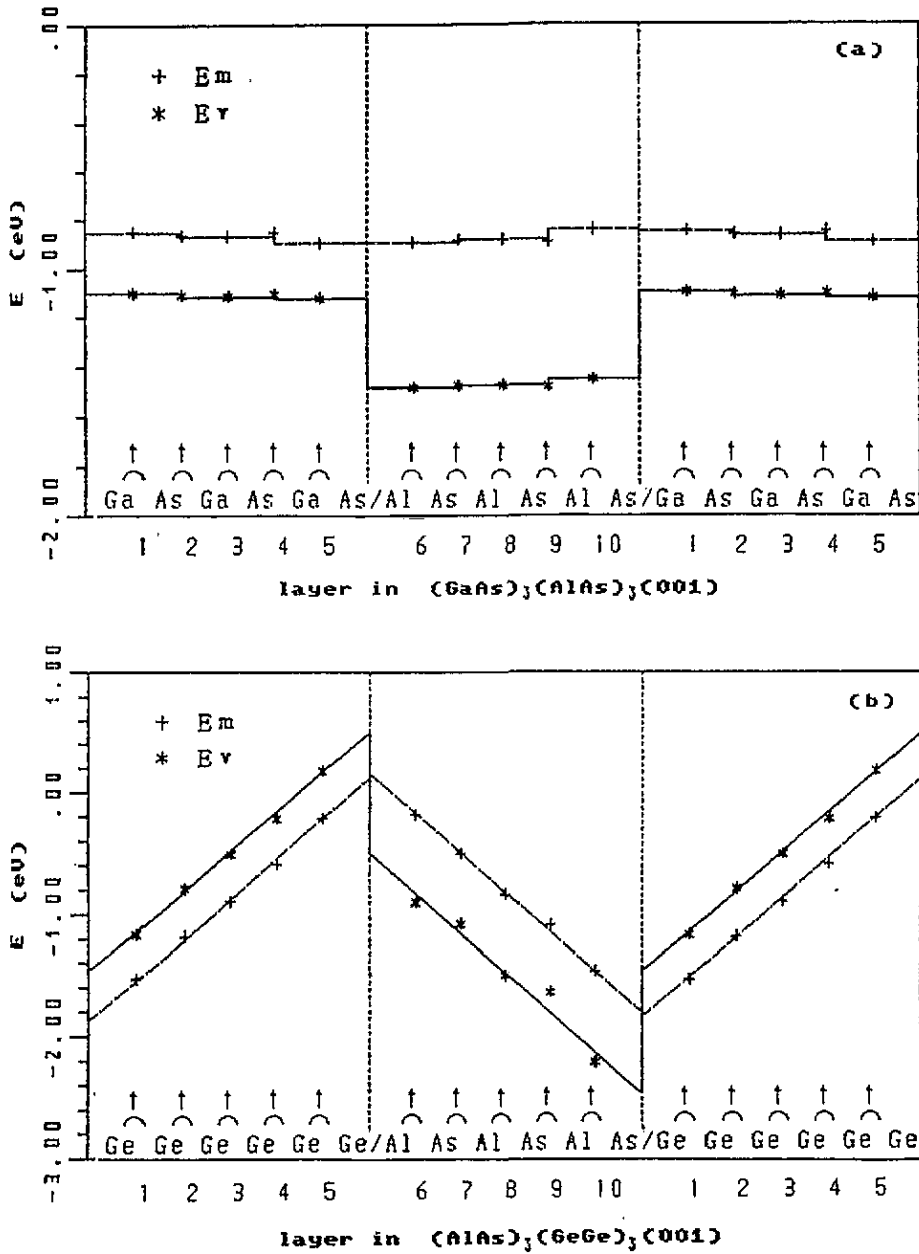


Figure 2. The valence band maximum E_v and average bond energy E_m in each molecular layer obtained by the frozen-potential treatment as mentioned in text: (a) $(\text{GaAs})_3(\text{AlAs})_3(001)$; (b) $(\text{AlAs})_3(\text{GeGe})_3(001)$.

Al and As) or the two molecular layers (GaAs and AlAs) which constitute the interface of the superlattice $(\text{GaAs})_3(\text{AlAs})_3(001)$ are listed in tables 2 and 3 together with the corresponding quantities in the bulk materials GaAs and AlAs. Similarly, tables 4 and

Table 1. The locations of atomic and empty spheres, and the atomic and molecular layers in the SL $(AB)_3(CD)_3(001)$.

| Atomic layer | Atomic sphere | Location ($\times \frac{1}{4}a$) | Empty sphere | Location ($\times \frac{1}{4}a$) | Molecular layer |
|--------------|---------------|------------------------------------|--------------|------------------------------------|-----------------|
| 1 | A | (0, 0, 0) | E_A | (0, 2, 0) | } → 1 |
| 2 | B | (1, 1, 1) | E_B | (-1, 1, 1) | } → 2 |
| 3 | A | (0, 2, 2) | E_A | (2, 2, 2) | } → 3 |
| 4 | B | (-1, 1, 3) | E_B | (1, 1, 3) | } → 4 |
| 5 | A | (0, 0, 4) | E_A | (0, 2, 4) | } → 5 |
| 6 | B | (1, 1, 5) | E_B | (-1, 1, 5) | |
| 7 | C | (0, 2, 6) | E_C | (2, 2, 6) | } → 6 |
| 8 | D | (-1, 1, 7) | E_D | (1, 1, 7) | } → 7 |
| 9 | C | (0, 0, 8) | E_C | (0, 2, 8) | } → 8 |
| 10 | D | (1, 1, 9) | E_D | (-1, 1, 9) | } → 9 |
| 11 | C | (0, 2, 10) | E_C | (2, 2, 10) | } → 10 |
| 12 | D | (-1, 1, 11) | E_D | (1, 1, 11) | |

5 contain the data for the four atomic layers (Ge, Ge, Al and As), the two molecular layers ($Ge\uparrow Ge$ and $Al\uparrow As$) and the interfaces of $(AlAs)_3(GeGe)_3(001)$. The excessive charge Δn in each molecular layer is shown in figure 1(a) for $(GaAs)_3(AlAs)_3(001)$ and figure 1(b) for $(AlAs)_3(GeGe)_3(001)$.

Table 2. Calculated interface charge transfer in $(GaAs)_3(AlAs)_3(001)$: the number of valence electrons in the atomic layers ($n(Ga)$, $n(As)$ and $n(Al)$) and molecular layers ($n(Ga+As)$ and $n(As+Al)$) for the $Ga\uparrow As/Al$ interface. The corresponding quantities in bulk materials are given in parentheses. Δn is the difference between the n -values of the SL and bulk.

| | $n(Ga)$ (electrons/layer) | $n(As)$ (electrons/layer) | $n(Al)$ (electrons/layer) | $n(Ga+As)$ (electrons/layer) | $n(As+Al)$ (electrons/layer) |
|--------------------|------------------------------|------------------------------|------------------------------|---------------------------------|---------------------------------|
| $Ga\uparrow As/Al$ | 3.130 | 4.963 | 2.945 | 8.093 | 7.908 |
| GaAs | (3.122) | (4.878) | | (8.000) | |
| AlAs | | (5.066) | (2.934) | | (8.000) |
| Δn | 0.008 | 0.085 | | 0.093 | |
| | | -0.103 | 0.011 | | -0.092 |

The frozen-potential treatment [10] is used to determine the valence band maximum E_v and the average bond energy E_m in each molecular layer of the SLS. In other words, we use the ASA potentials of atomic spheres and empty spheres contained in molecular layers AB or CD in $(AB)_3(CD)_3(001)$ obtained by self-consistent calculation as input to determine directly the band structures of the bulk material AB or CD. Then, the bonding energy E_b , anti-bonding energy E_a and average bond energy E_m in each molecular layer can be expressed as [11, 12]

$$E_b = \frac{1}{4N} \sum_{n=1}^4 \sum_k E_n(k) \quad (5)$$

Table 3. Calculated interface charge transfer in (GaAs)₃(AlAs)₃(001): results for the Al Γ As/Ga interface. The notation is similar to that in table 2.

| | $n(\text{Al})$ (electrons/layer) | $n(\text{As})$ (electrons/layer) | $n(\text{Ga})$ (electrons/layer) | $n(\text{Al+As})$ (electrons/layer) | $n(\text{As+Ga})$ (electrons/layer) |
|-------------------|-------------------------------------|-------------------------------------|-------------------------------------|--|--|
| Al Γ As/Ga | 2.943 | 4.965 | 3.128 | 7.908 | 8.093 |
| AlAs | (2.934) | 5.066) | | (8.000) | |
| GaAs | | (4.878 | 3.122) | | (8.000) |
| Δn | 0.009 | -0.101 0.087 | 0.006 | -0.092 | 0.093 |

Table 4. Calculated interface charge transfer in (AlAs)₃(GeGe)₃(001): results for the Ge Γ Ge/Al Γ As interface. The notation is similar to that in table 2.

| | $n(\text{Ge})$ (electrons /layer) | $n(\text{Ge})$ (electrons /layer) | $n(\text{Al})$ (electrons /layer) | $n(\text{As})$ (electrons /layer) | $n(\text{Ge+Ge})$ (electrons /layer) | $n(\text{Al+As})$ (electrons /layer) |
|-------------------------------|---|---|---|---|--|--|
| Ge Γ Ge/Al Γ As | 3.999 | 4.067 | 2.961 | 5.042 | 8.066 | 8.003 |
| Ge | (4.000 | 4.000) | | | (8.000) | |
| AlAs | | | (2.934 | 5.066) | | (8.000) |
| Δn | -0.001 | 0.067 | 0.027 | -0.024 | 0.066 | 0.003 |

Table 5. Calculated interface charge transfer in (AlAs)₃(GeGe)₃(001): results for the Al Γ As/Ge Γ Ge interface. The notation is similar to that in table 2.

| | $n(\text{Al})$ (electrons /layer) | $n(\text{As})$ (electrons /layer) | $n(\text{Ge})$ (electrons /layer) | $n(\text{Ge})$ (electrons /layer) | $n(\text{Al+As})$ (electrons /layer) | $n(\text{Ge+Ge})$ (electrons /layer) |
|-------------------------------|---|---|---|---|--|--|
| Al Γ As/Ge Γ Ge | 2.953 | 4.995 | 3.979 | 4.010 | 7.948 | 7.909 |
| AlAs | (2.934 | 5.066) | | | (8.000) | |
| Ge | | | (4.000 | 4.000) | | (8.000) |
| Δn | 0.019 | -0.071 | -0.021 | 0.010 | -0.052 | -0.011 |

$$E_a = \frac{1}{4N} \sum_{n=5}^8 \sum_k E_n(\mathbf{k}) \quad (6)$$

$$E_m = \frac{1}{2}(E_b + E_a). \quad (7)$$

Here, N is the number of unit cells and $E_n(\mathbf{k})$ the eigenvalue of the n th band. The E_v - and E_m -values in each molecular layer are shown in figure 2. Tables 6 and 7 list the E_v - and E_m -values in the two interface molecular layers.

3. Discussion

3.1. Structural comparison between common-anion and non-common-ion heterojunctions

The interface of the common-anion SL is different from that of the non-common-ion SL. For the common-anion SL (GaAs)₃(AlAs)₃(001) (figure 1(a)), the two atomic layers As/Al or

Table 6. Valence band maxima E_v and average bond energies E_m in bulk materials and in the molecular layer beside the SL interfaces in $(\text{GaAs})_3(\text{AlAs})_3(001)$.

| | Bulk materials | | | The two interfaces in $(\text{GaAs})_3(\text{AlAs})_3(001)$ | | | | | |
|------------|----------------|-------|------------|---|--------------|------------|--------------|--------------|------------|
| | | | | 5 | | 6 | | 10 | |
| | GaAs | AlAs | ΔE | Ga \cap As | Al \cap As | ΔE | Al \cap As | Ga \cap As | ΔE |
| E_m (eV) | -1.07 | -0.65 | -0.42 | -0.89 | -0.89 | 0.00 | -0.84 | -0.85 | -0.01 |
| E_v (eV) | -1.30 | -1.23 | -0.07 | -1.12 | -1.49 | 0.37 | -1.46 | -1.10 | 0.36 |

Table 7. Valence band maxima E_v and average band energies E_m in bulk materials and in the molecular layer beside the SL interfaces in $(\text{AlAs})_3(\text{GeGe})_3(001)$.

| | Bulk materials | | | The two interfaces in $(\text{AlAs})_3(\text{GeGe})_3(001)$ | | | | | |
|------------|----------------|-------|------------|---|--------------|------------|--------------|--------------|------------|
| | | | | 5 | | 6 | | 10 | |
| | GeGe | AlAs | ΔE | Ge \cap Ge | Al \cap As | ΔE | Al \cap As | Ge \cap Ge | ΔE |
| E_m (eV) | -0.96 | -0.65 | -0.31 | -0.21 | -0.18 | -0.03 | -1.47 | -1.53 | -0.06 |
| E_v (eV) | 0.57 | -1.23 | 0.66 | 0.18 | -0.90 | 1.08 | -2.21 | -1.17 | 1.05 |

As/Ga on the two sides of the interface constitute the molecular layer across the interface, i.e. the interface molecular layer, which is chemically the same as the bulk constituents AlAs or GaAs. However, in the non-common-ion SL $(\text{AlAs})_3(\text{GeGe})_3(001)$ the two interface molecular layers Ge/Al and As/Ge are chemically different from the two bulk constituents AlAs and Ge. Consequently, for the common-anion SL the As atomic layer at the interface Ga \cap As/Al can be considered to be used commonly by the molecular layers Ga \cap As and As/Al and to become almost the 'real interface' of the SL. On the other hand, in the non-common-ion SL the molecular layer Ge/Al at the interface Ge \cap Ge/Al \cap As is chemically different from the two bulk constituents AlAs and Ge. As a result, the 'real interface' of the non-common-ion SL is between the two molecular layers Ge \cap Ge and Al \cap As. For the reason mentioned above, the two molecular layers near the interface in the common-anion SL consist of three atomic layers, while those in the non-common-ion SL contain four atomic layers. This difference in the interface structure results in the different behaviours of interface charge transfer and other relevant behaviours in these two kinds of SL.

3.2. The interface charge transfer in superlattices

It can be seen in table 2 that, for the common-anion SL, the $n(\text{As})$ -value of the interface As atomic layers (4.963) is close to the average of those in the two bulk constituents (4.878 and 5.066); the relative changes are 0.085 and -0.103 , respectively. The $n(\text{Ga})$ - and $n(\text{Al})$ -values in the SL are also different from those in the bulk (Δn equal to 0.008 and 0.001, respectively), but they are much smaller than $\Delta n(\text{As})$. In table 2, $\Delta n(\text{Ga} + \text{As}) = 0.093$ and $\Delta n(\text{As} + \text{Al}) = -0.092$ imply a dipole between the two molecular layers Ga \cap As and As/Al. The charge of this dipole is mainly due to $\Delta n(\text{As})$. In the case of Al \cap As/Ga, the situation is very similar (see table 3).

In table 4, it appears that in the non-common-anion SL the charge neutral deviation in Ge \cap Ge/Al \cap As is 0.066 for Ge \cap Ge and 0.003 for Al \cap As. Although the two values are obviously different, their sign is the same; consequently, no dipole exists at the Ge \cap Ge/Al \cap As interface. The situation at the Al \cap As/Ge \cap Ge interface is similar (see table 5).

The conditions of excessive charge distributions in the two kinds of SL are shown in figures 1(a) and 1(b). It is obvious that the redistribution of valence electrons takes place mainly in the two molecular layers beside the interface; the molecular layers far from the interface remain almost neutral. The difference between the common-ion SL and the non-common-anion SL is that, in the former, there is an interface dipole but, in the latter, there is a monopole.

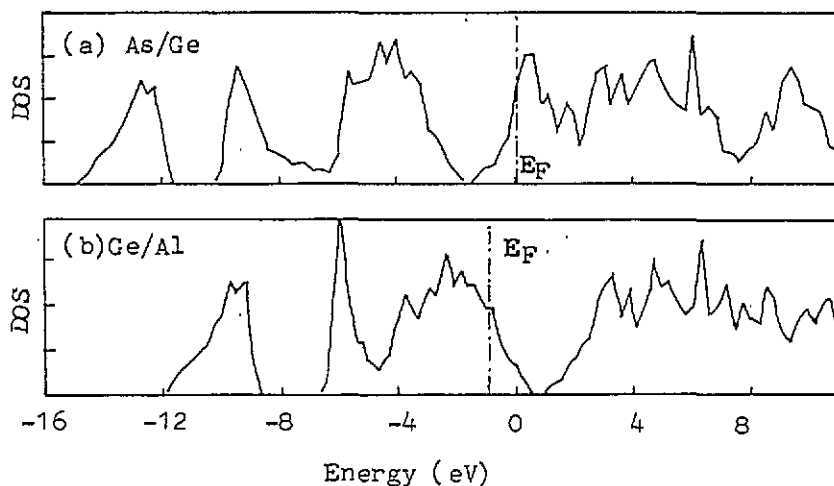


Figure 3. Density of states and Fermi level of the interface molecular layer in the SL $(\text{AlAs})_3(\text{GeGe})_3(001)$, obtained by using the self-consistent bulk charge density as the input: (a) $E_F(\text{As/Ge})=0.31$ eV; (b) $E_F(\text{Ge/Al})=-1.35$ eV.

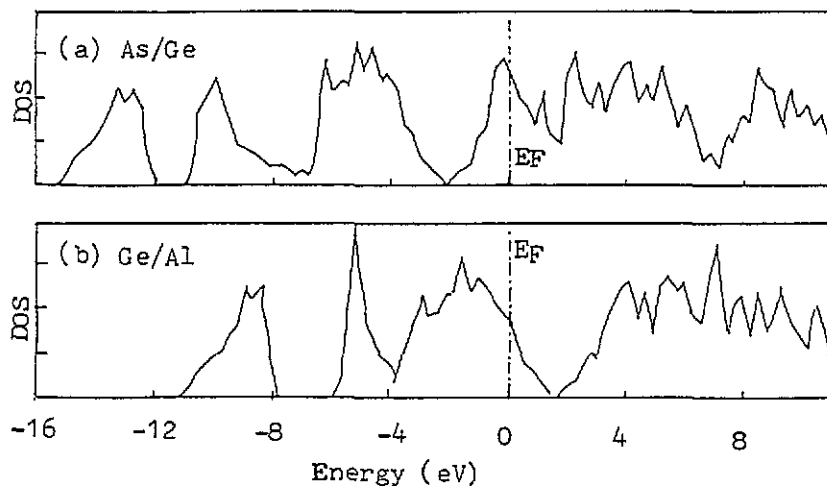


Figure 4. Density of states and Fermi level of the interface molecular layer in the SL $(\text{AlAs})_3(\text{GeGe})_3(001)$, obtained by using the self-consistent SL charge density as the input: (a) $E_F(\text{As/Ge})=-0.31$ eV; (b) $E_F(\text{Ge/Al})=-0.49$ eV.

3.3. The valence band offset and the internal electric field in SLs

In figure 2 the valence band edges of the two SLs appear as a discontinuous step at the interfaces, i.e. the valence band offset ΔE_v , while the average bond energy E_m is aligned across the interfaces (their values are listed in tables 6 and 7), and this justifies E_m as a reasonable reference level for determining the ΔE_v -value in heterostructures [13]. Comparing figure 2 with figure 1, one can see that the alignment of the average bond energy E_m across the interfaces is determined by the interface charge transfer as shown in our previous work [14] but has nothing to do with whether the interface dipole exists. In figure 2 the curve of E_v is always parallel to the curve of E_m ; their slope reflects the strength of the internal electric field in the SL layers. In the common-anion SL this slope equals zero; so there is no internal electric field in the SL layers; the situation in the non-common-ion SL is contrary to this. This can be understood by analysing the distribution of excessive charge among different molecular layers. In the common-anion SL the numbers of interface dipoles at two adjacent interfaces (Ga \cap As/Al and Al \cap As/Ga) are the same but their signs are opposite; their roles cancel out and vanish in bulk-like SL layers; thus there is no internal electric field in this region. In the non-common-ion SL, molecular layers at the Ge \cap Ge/Al \cap As interface have a negative excessive charge, while those at the Al \cap As/Ge \cap Ge interface have a positive excessive charge (figure 1(b)); the result is an internal electric field in the bulk-like SL layers.

By summing the Δn -values of every atomic layer in Ge \cap Ge/Al \cap As (listed in table 4), one obtains $\Delta Q = 0.069$ which corresponds to a charge face density $\sigma = 0.069 \text{ C m}^{-2}$. Using the expression for two parallel capacitor plates charged with σ electrons per unit area, one can find the strength of the internal electric field $E = 2.23 \times 10^9 \text{ V m}^{-1}$ with the dielectric constant $\epsilon = 3.5$ resulting from microscopic calculations for the interfaces in [15]. On the other hand, the strength of the internal electric field determined directly from the slope of the E_v or E_m curve drawn in figure 2(b) is $E = 2.3 \times 10^9 \text{ V m}^{-1}$. The two results are perfectly consistent with each other. The magnitude of this electric field is the same as those in the SL Ge/GaAs(001) (about 10^9 V m^{-1}) [16].

4. Charge transfer between interface molecular layers and the location of the Fermi level

In tables 4 and 5, it appears that the excessive charge occurs in the interface molecular layers Ge/Al and Al/Ge: $\Delta n(\text{Ge}) + \Delta n(\text{Al}) = 0.094$; $\Delta n(\text{As}) + \Delta n(\text{Ge}) = -0.092$. About 0.09 electrons are transferred from the As/Ge molecular layer to the Ge/Al molecular layer. In order to investigate the effect of this charge transfer, we have calculated the density of states and Fermi level for the interface molecular layers As/Ge and Ge/Al contained in (AlAs)₃(GeGe)₃(001), using the self-consistent charge density of bulk Ge, AlAs and SL (AlAs)₃(GeGe)₃(001) as the inputs, respectively. The effect of the charge transfer is included in the latter case (using the self-consistent SL charge density as the input) but not in the former case (using the self-consistent bulk charge density as the input). The calculated results in the two cases are shown in figure 3 and figure 4, respectively. In figures 3(a) and 3(b) and in figures 4(a) and 4(b), one can see that the locations of two Fermi levels are obviously different (0.36 eV and -1.34 eV , respectively, i.e. different by 1.70 eV). When the interface charge transfer is included, the two Fermi levels become very close to each other (-0.32 eV and -0.53 eV , respectively, i.e. different by 0.21 eV; see figure 4). The change in the difference between the two Fermi levels induced by the charge transfer is 1.49 eV which is fairly consistent with the magnitude of the potential barrier height of the

internal electric field (see figure 2(b)). This indicates that the interface molecular layers (possessing the characteristic of a metal) are different from the bulk-like molecular layers. The difference between the states of As/Ge and Ge/Al is the main factor leading to the internal electric field in the non-common-ion SL.

In summary, our calculations for the two kinds of SL show that the internal electric field depends on the interface structure; this field exists in the non-common-ion SL but does not in the common-anion SL. Of course, the interface structures studied above are ideal interfaces. If non-ideal factors, such as the interdiffusion of different atoms at the interface, are considered, the internal electric field will be reduced or eliminated [1].

Acknowledgments

The authors thank the Computing Centre of Xiamen University for providing research facilities. This work was supported by the National Science Foundation of China and the Natural Science Foundation of Fujian Province.

References

- [1] Harrison W A, Kraut E A, Waldrop J R and Grant R W 1978 *Phys. Rev. B* **18** 4402
- [2] Eppenga R 1989 *Phys. Rev. B* **40** 10402
- [3] Skriver H L 1984 *The LMTO Method* (Berlin: Springer) p 62
- [4] Lambrecht W R and Andersen O K 1986 *Phys. Rev. B* **34** 2439
- [5] Wang R Z and Huang M C 1990 *Comput. Phys.* **7** 85
- [6] Wang R Z and Huang M C 1990 *Acta Phys. Sin.* **39** 1135
- [7] Wu S T, Wang R Z and Zheng Y M 1992 *J. Xiamen Univ. (Natural Sci. Edition)* **31** 487
- [8] Chadi D J and Cohen M L 1973 *Phys. Rev. B* **8** 5747
- [9] Cunningham S L 1974 *Phys. Rev. B* **10** 4988
- [10] Christensen N E 1988 *Phys. Rev. B* **37** 4528
- [11] Chen A B 1981 *Phys. Rev. B* **23** 5360
- [12] Wang R Z and Huang M C 1991 *Acta Phys. Sin.* **40** 1683
- [13] Wang R Z, Huang M C and Ke S H 1992 *Sci. China (Ser. A)* **36** 45
- [14] Wang R Z, Ke S H and Huang M C 1992 *J. Phys. C: Solid State Phys.* **4** 8083
- [15] Flores F and Tejedor C 1979 *J. Phys. C: Solid State Phys.* **12** 731
- [16] Bylander D M and Kleinman L 1990 *Phys. Rev. B* **41** 3509