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Band line-ups and band-gap behaviour of new-type superlattices (3C-BN)/(2H-BN), (3C-GaN)/(2H-GaN) and (3C-SiC)/(2H-SiC)

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Abstract. We report *ab initio* calculations of the electronic structures and the band line-ups of heterocrystalline superlattices (HSLs) $(3\text{C-BN})_{3n}/(2\text{H-BN})_{2n}$, $(3\text{C-GaN})_{3n}/(2\text{H-GaN})_{2n}$ and $(3\text{C-SiC})_{3n}/(2\text{H-SiC})_{2n}$ ($n = 1, 2, 3$). The band line-ups at both the $(3\text{C-BN})/(2\text{H-BN})$ interface and the $(3\text{C-SiC})/(2\text{H-SiC})$ interface are found to be type II, with valence-band offsets of 0.16 eV and 0.14 eV and conduction-band offsets of up to 1.56 eV and 1.08 eV respectively. For the $(3\text{C-GaN})/(2\text{H-GaN})$ interface, the valence-band offset is found to be almost zero, and the conduction-band offset is about 0.4 eV. It is found that the band gaps in the HSLs decrease rapidly with the increase of the slab thickness. This 'abnormal' band-gap behaviour is shown to be due to the internal electric fields induced by the spontaneous polarizations in the 2H structures.

1. Introduction

Recently, several theoretical studies [1–3] have been devoted to a new group of superlattices (denoted as heterocrystalline superlattices (HSLs) hereafter), which are formed by two chemically identical but structurally different materials, namely by the polytypes of a material. SiC is a typical material which exhibits pronounced polytypism. It crystallizes in more than 100 different crystalline modifications. The two most extreme polytypes are zincblende (3C) with pure cubic stacking of the Si–C bilayers in the [111] direction and wurtzite (2H) with pure hexagonal stacking in the [0001] direction. For this reason, SiC has been studied [2, 3] as a typical material for forming HSLs. Besides SiC, the II–VI compounds ZnS [4] and CdS [5] also exist in many polytypes, typically in the 3C structure and the 2H structure. However, the electronic band structures of these polytypes are found to be very similar and the difference in band gaps is less than 0.1 eV. So the band offsets at the interfaces of the HSLs formed by these polytypes are negligible. On the other hand, although the stable phase of III–V compounds BN, AlN and GaN bulk materials have the 3C structure (for BN) and 2H structure (for GaN and AlN), 2H structural BN and 3C structural AlN, GaN have also been experimentally observed and their properties are beginning to be measured. These advances have come largely as a result of improved crystal growth techniques, such as the molecular-beam epitaxy (MBE) technique. So far, the pure HSLs formed by these polytypes have still not been successfully fabricated in a controlled manner, and it seems to be hard to grow two polytypes together to form a pure HSL using the experimental techniques currently available. However, because of the small

energy differences between polytypes of a material (see, for example, [6]), single-phase films are difficult to make, and the polytype selection is likely to be dominated by kinetic factors. Under this condition, the interfaces in the pure HSL will occur as defects in mixed polytype films. So, it is still very interesting to see how the two band structures line up at the interfaces of the pure HSL. Also very interesting is the effect of the spontaneous polarizations in the 2H compounds on the electronic properties of the HSLs. In this paper, we report *ab initio* calculations of the electronic structures and band offsets of the HSLs $(3\text{C-BN})_{3n}/(2\text{H-BN})_{2n}$, $(3\text{C-GaN})_{3n}/(2\text{H-GaN})_{2n}$ and $(3\text{C-SiC})_{3n}/(2\text{H-SiC})_{2n}$ ($n = 1, 2, 3$) grown in the $[111]$ – $[0001]$ direction. The slab-thickness dependence of the band gaps in the HSLs and its relation with the effects of spontaneous polarizations in the 2H compounds are discussed.

2. Computational details

2.1. Structural details

It is well known that the 3C structure has a pure cubic stacking of the anion–cation (such as N–B, N–Ga and C–Si) bilayers in the $[111]$ direction, whereas the 2H structure has a pure hexagonal stacking of the bilayers in the $[0001]$ direction. The stacking of bilayers in a unit cell is commonly described as ABC for the 3C structure and AB for the 2H structure. In the $[111]$ – $[0001]$ direction, the two structures can be grown together to form a ‘heterostructure’. The positions of atoms in the 3C structure and the 2H structure, as well as in the HSLs are shown in figure 1.

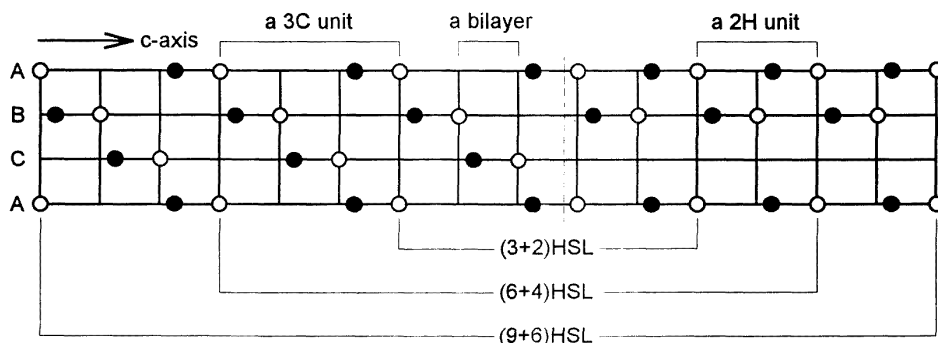


Figure 1. The projected positions of atoms upon the $(11\bar{2}0)$ plane in the HSLs under consideration. The circles and the dots represent, respectively, the anion and cation atoms in a compound. The different $(\bar{1}100)$ planes within the unit cells are denoted by A, B and C to make obvious the stacking sequence.

For the 2H structure, there are three independent structural parameters, which are usually taken as the lattice constant a normal to the stacking direction, the ratio of c/a (with c being the lattice constant along the stacking direction) and the internal relaxation parameter u , which is defined as d/c where d is the length of the bond along the stacking direction. The ideal values of c/a and u are 1.6330 and 0.3750 respectively. The experimental data [7] of u and c/a for 2H-BN, 2H-GaN and 2H-SiC are fairly close to the ideal values. In this work, the ideal values are adopted, and the bond lengths of the 3C–2H compound pair

are taken to be the same. The structural parameters are listed in table 1.

Table 1. The lattice constants (from [7]) and minimum corrected band gaps (in eV) of 3C-BN, 2H-BN, 3C-GaN and 2H-GaN (from [10]) and the experimental band gaps (in eV) of 3C-SiC and 2H-SiC (from [11]).

	3C-BN	2H-BN	3C-GaN	2H-GaN	3C-SiC	2H-SiC
a (Å)	3.68	2.56	4.51	3.19	4.36	3.08
c (Å)		4.18		5.21		5.05
E_g	6.4	7.8	3.24	3.65	2.39	3.33
	$(E_c^X - E_v^I)$	$(E_c^K - E_v^I)$	$(E_c^F - E_v^I)$	$(E_c^F - E_v^I)$	$(E_c^X - E_v^I)$	$(E_c^K - E_v^I)$

2.2. Details of the calculations for band structures and band offsets

In this work, the linear muffin-tin orbitals (LMTO) method within the atomic-sphere approximation (ASA) is used to perform the self-consistent calculations for the 3C compounds, the 2H compounds and the HSLs. This method is based on the density functional theory (DFT) in the local density approximation (LDA). For the integration over k space, three special k points in the irreducible Brillouin zone are used. An internal summation approach [8] is adopted to the higher-energy and unoccupied d orbitals. For the calculations of the GaN HSLs, the 3d orbitals of the Ga atom are taken as the valence-band states, since their LDA eigenvalues overlap with the N 2s bands and were found to be important for obtaining correct ground-state charge densities.

As usual, the so-called ‘empty spheres’ are added into the interstitial regions in the lattices of both the 3C and the 2H structures. In the case of 3C structure, all the empty spheres have the same radius, which is taken to be the same as that of atomic spheres (denoted by r_a). For the 2H structure, the situation is somewhat more complicated, since there are two different kinds of interstitial region in its lattice. In this work, the total volume of atomic spheres in the 2H structure is chosen to be 50% of the volume of the unit cell, as in the case of 3C structure, and the radii of the two kinds of empty sphere (denoted by r_{e1} and r_{e2} respectively) are carefully optimized so that the two kinds of empty sphere overlap evenly with their nearest-neighbouring atomic spheres. The optimized result is $r_a : r_{e1} : r_{e2} = 1 : 1.177 : 0.718$.

The band offsets at the HSL interfaces are determined using a frozen-potential method, which is described below. In the LMTO-ASA method, the energy-band problem can be separated into a potential-dependent part which is represented by the values of four potential parameters on the surface of a muffin-tin sphere, and a crystal-structure-dependent part which is represented by the structure constants. Through self-consistent supercell calculations, we can obtain the self-consistent potential parameters for each atomic sphere and each empty sphere in an HSL. Then, the potential parameters can be divided into two groups which correspond to the two material layers in the supercell. By using the two groups of potential parameter as the final inputs, one can solve the secular matrix for the two bulk materials separately, and obtain their valence-band maxima (VBM). Finally, the valence-band offset (VBO) at the HSL interface can be determined by comparing the two VBM of the two material layers. In practice, the self-consistent potential parameters of the two central bilayers in the two slabs of an HSL are adopted to determine the VBO at the interface.

3. Results and discussions

3.1. Band offsets

Considering the convergence problem with the frozen potential calculations for band offsets, we have performed the frozen potential calculations using the self-consistent potential parameters obtained from the self-consistent supercell calculations for $(3\text{C-BN})_{3n}/(2\text{H-BN})_{2n}$, $(3\text{C-GaN})_{3n}/(2\text{H-GaN})_{2n}$, and $(3\text{C-SiC})_{3n}/(2\text{H-SiC})_{2n}$ ($n = 1, 2, 3$). The results are listed in table 2. Our calculations show that the conduction-band minima (CBM) of 3C-BN and 3C-SiC are at the X point of the zincblende Brillouin zone, the CBM of 2H-BN and 2H-SiC are at the K point of the wurtzite Brillouin zone, and both 3C-GaN and 2H-GaN are direct band-gap (at the Γ point) semiconductors.

Physically, the band offsets at a heterointerface generally relate to the valence bands and conduction bands of the two constituents for large layer thickness. In the case of short-period superlattice interfaces the interaction between electronic states modifies the band structures with respect to the thick layer limit. This leads to the convergence problem with *ab initio* supercell calculations for band offsets. However, it appears in table 2 that the VBOs calculated using the self-consistent potential parameters of the $(3 + 2)$ HSLs and $(9 + 6)$ HSLs are very close to each other. The largest difference is only 0.01 eV. This indicates that for HSLs the bulk property of bilayers is almost recovered even in the smallest HSL system. This behaviour is due to the identical chemical character on the two sides of the HSL interfaces.

All of the VBOs at the $(3\text{C-BN})/(2\text{H-BN})$, $(3\text{C-GaN})/(2\text{H-GaN})$ and $(3\text{C-SiC})/(2\text{H-SiC})$ interfaces turn out to be fairly small (0.16 eV, 0.01 eV and 0.14 eV respectively). This is understandable since the bond characters on the two sides are almost the same. The present result for the $(3\text{C-SiC})/(2\text{H-SiC})$ interface (0.14 eV) is in very good agreement with the result of 0.13 eV obtained from the *ab initio* pseudopotential calculation in [3]. The relative values of the VBO between the three HSL interfaces given by our calculations are also consistent with the conclusion reached in [1], which states that the value of the VBO at an HSL interface increases with the decrease of the ionicity of the bond.

A factor which influences the accuracy of the above LDA-derived band offsets is the quasi-particle (QP) correction to LDA band gaps. However, for the majority of heterointerfaces the influence of the QP correction on the VBO, which is really a ground-state property, is fairly small. The work by Zhu and Louie [9] has shown that typical values are around 0.1 eV. In the case of HSLs, the QP effects seem to be smaller. For SiC, the work by Bechstedt and Kackell [3] showed that the maximum variation of the gap opening with the polytype is about 0.1 eV or even smaller. Despite this, in order to obtain reliable values of the conduction-band offset (CBO) at the HSL interfaces, in this work we use the data of corrected band gaps reported in [10], except for the $(3\text{C-SiC})/(2\text{H-SiC})$ interface whose CBO is obtained using experimental band-gap data [11] (2.39 eV for 3C-SiC and 3.33 for 2H-SiC). For a number of semiconductors, these data appear to be in good agreement with experimental values of band gaps. The corrected band gaps are 6.4 eV, 7.8 eV, 3.24 eV and 3.65 eV for 3C-BN, 2H-BN, 3C-GaN and 2H-GaN respectively (see table 1). By adding the difference in the band gaps into the VBO, we obtain CBO values of 1.56 eV ($E_v^K(2\text{H}) - E_v^X(3\text{C})$) for $(3\text{C-BN})/(2\text{H-BN})$, 0.40 eV ($E_v^\Gamma(2\text{H}) - E_v^\Gamma(3\text{C})$) for $(3\text{C-GaN})/(2\text{H-GaN})$, and 1.08 eV ($E_v^K(2\text{H}) - E_v^X(3\text{C})$) for $(3\text{C-SiC})/(2\text{H-SiC})$. It appears that the band line-ups at the $(3\text{C-BN})/(2\text{H-BN})$ and $(3\text{C-SiC})/(2\text{H-SiC})$ interfaces are type II with small VBOs and large CBOs. So, the valence electrons will be confined strongly in the 3C-BN and 3C-SiC slabs. On the other hand, the VBO at the $(3\text{C-GaN})/(2\text{H-GaN})$

Table 2. The calculated band offsets and minimum LDA band gaps (in eV) of the HSLs. $\Delta E_g = E_g - E_g(3+2)$ HSL is the change in band gap with respect to the (3+2) HSL due to the increase of the slab thickness, obtained from the self-consistent calculations. $\Delta E'_g$ is the corresponding quantity to ΔE_g but is obtained from equation (2). IEF = $\partial \text{VBM} / \partial z$ is the slope of the VBM along the normal direction (in units of V \AA^{-1} .)

(3C-BN)/(2H-BN)			
	(3+2)	(6+4)	(9+6)
VBO [$E_v^\Gamma(2\text{H}) - E_v^\Gamma(3\text{C})$]	0.15	0.16	0.16
CBO [$E_c^K(2\text{H}) - E_c^K(3\text{C})$]	1.55	1.56	1.56
E_g	5.10 ^a	4.20 ^b	3.30 ^b
ΔE_g	0.00	-0.90	-1.80
$\Delta E'_g$	0.00	-0.93	-1.86
IEF		-0.148, 0.222	-0.147, 0.221
(3C-GaN)/(2H-GaN)			
	(3+2)	(6+4)	(9+6)
VBO [$E_v^\Gamma(2\text{H}) - E_v^\Gamma(3\text{C})$]	0.02	0.01	0.01
CBO [$E_c^\Gamma(2\text{H}) - E_c^\Gamma(3\text{C})$]	0.39	0.40	0.40
E_g	2.57 ^c	1.92 ^c	1.27 ^c
ΔE_g	0.00	-0.65	-1.30
$\Delta E'_g$	0.00	-0.65	-1.30
IEF		-0.083, 0.126	-0.083, 0.125
(3C-SiC)/(2H-SiC)			
	(3+2)	(6+4)	(9+6)
VBO [$E_v^\Gamma(2\text{H}) - E_v^\Gamma(3\text{C})$]	0.14	0.14	0.14
CBO [$E_c^K(2\text{H}) - E_c^K(3\text{C})$]	1.08	1.08	1.08
E_g	1.99 ^a	1.40 ^b	0.81 ^b
ΔE_g	0.00	-0.59	-1.18
$\Delta E'_g$	0.00	-0.59	-1.18
IEF		-0.078, 0.118	-0.077, 0.116
$E_g(\text{relaxed})$	1.96 ^a	1.36 ^b	0.75 ^b
$\Delta E_g(\text{relaxed})$	0.00	-0.60	-1.22
$\Delta E'_g(\text{relaxed})$	0.00	-0.59	-1.18
IEF(relaxed)		-0.079, 0.115	-0.081, 0.112

^a Band gap of $L_c-\Gamma_v$.
^b Band gap of $L_c, M_c-\Gamma_v$.
^c Band gap of $\Gamma_c-\Gamma_v$.

interface is almost zero, and the CBO is also fairly small, since the band gaps in both 3C-GaN and 2H-GaN are direct and very close to each other.

3.2. Band-gap behaviour

For (3C-BN)/(2H-BN) and (3C-SiC)/(2H-SiC) systems, since the band line-ups are of type-II character, a band gap in each of them is expected which mainly arises from the narrow-band-gap constituent (namely the 3C-BN and 3C-SiC respectively), but is reduced by the amount of the VBO. On the other hand, the band gap in the (3C-GaN)/(2H-GaN) system is expected to be between those of 3C-GaN and 2H-GaN, since the VBO is almost zero.

However, from the calculated values of the band gaps in the HSLs (see table 2), one can see that the situation is not as expected. The band gaps of the HSLs turn out to decrease rapidly with the increase of the slab thickness, and the amount of the decrease is proportional to the slab thickness. For the $(3\text{C-SiC})_{3n}/(2\text{H-SiC})_{2n}$ system, we find that in the case of $n \geq 2$ the band gap is already smaller than the smallest band gap in the constituents (namely the band gap in 3C-SiC). The phenomenon that the LDA band gap of an HSL is smaller than the smallest LDA band gap in the constituents was also found for $(3\text{C-SiC})/(2\text{H-SiC})$ in [3], where it was regarded as an astonishing phenomenon since it cannot be ascribed only to the type II band-line-up character. In this paper, we show that this ‘abnormal’ band-gap behaviour is due to the macroscopic internal electric fields (IEFs) induced by the spontaneous polarizations in the 2H structures.

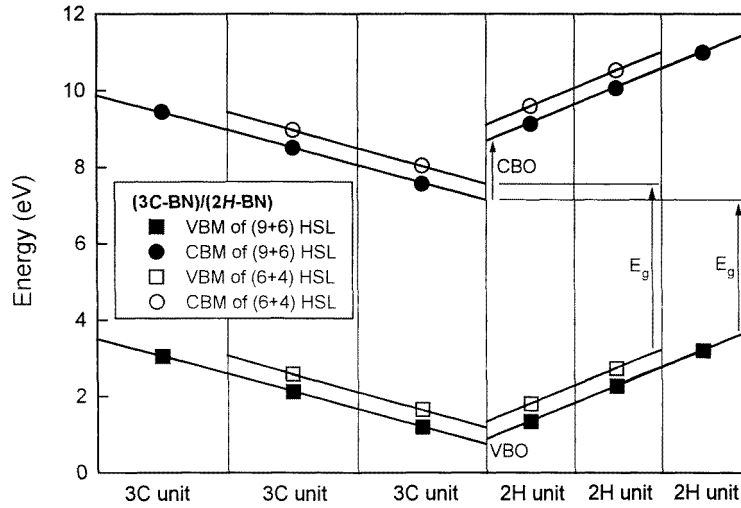
Compared with the 3C structure, the 2H structure has a lower symmetry. As a result, it is expected to possess a spontaneous polarization: since the four tetrahedral bonds are no longer equivalent, bond-to-bond charge transfer and ionic relaxation may cause the spontaneous polarization along the stacking direction. The spontaneous polarization leads to an electric potential difference between the two ends of a finite crystal, along the polarization axis. In the case of an HSL in the form of 3C–2H, the spontaneous polarization in the 3C slab is zero by symmetry, so the spontaneous polarization in the 2H slab will lead to a macroscopic IEF in both the 3C slab and the 2H slab. This IEF will change the energies of the band extremes in real space and reduce the band gap of the HSL. Obviously, the amount of this reduction is proportional to the slab thickness, as we can see from table 2.

In order to show directly the IEF and its relation with the ‘abnormal’ band-gap behaviour, we have performed further frozen potential calculations for the three HSLs. In an HSL supercell of form $(3\text{C})_{3n}/(2\text{H})_{2n}$, the 3C slab contains n unit cells of the 3C compound and the 2H slab contains n unit cells of the 2H compound. Therefore, we can divide the supercell of the HSL into n 3C units and n 2H units (see figure 1). The VBM of each 3C unit or 2H unit can then be calculated by the frozen-potential method using the self-consistent potential parameters of each 3C unit or 2H unit. The line-ups of the VBMs of the n 3C units and the n 2H units will give us information about the distribution of the average electric potential along the normal direction. The calculated results are shown in figure 2. The scissors corrections to the LDA band gaps are already included in figure 2.

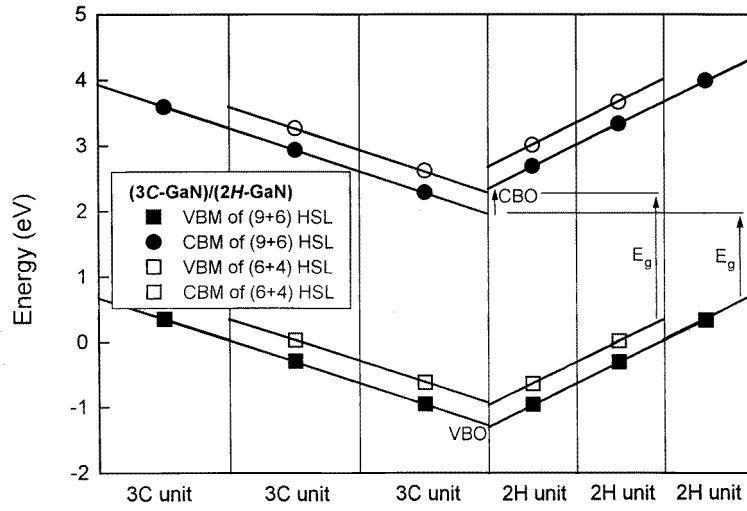
From figure 2 it can be seen that in both the 3C slab and the 2H slab the value of VBM (or CBM) is remarkably different for different positions of the 3C unit or 2H unit. The slope of the VBM (or the CBM) is related to the macroscopic IEFs. One may consider that the IEFs are partly created from the piezoelectricity. It should be noted that the HSLs studied here are lattice-matched and the structure parameters used for the wurtzite constituents are the ideal values, which agree well with the experimental values and can also be expected to be fairly close to the theoretical equilibrium lattice parameters obtained from total energy minimization calculations (for SiC, see [3]). So, the piezoelectric effect in the present case can be expected to be fairly small. From figure 2 one can find that the IEFs in $(6+4)$ HSLs are almost the same as those in the $(9+6)$ HSLs, which indicates that quantum size effects here are also fairly small. The IEFs can be therefore mainly ascribed to the spontaneous polarization in the 2H slabs. Following this train of thought, the band gap in an HSL will really decrease proportionally with the increase of the slab thicknesses. If the VBOs at the two interfaces of the HSL are assumed to be exactly the same, then we have

$$\Delta E_g = -d(3\text{C}) \times \text{IEF}(3\text{C}) = -d(2\text{H}) \times \text{IEF}(2\text{H}) \quad (1)$$

where $\text{IEF} = \partial \text{VBM} / \partial z$ (its values are listed in table 2), the $d(3\text{C})$ and $d(2\text{H})$ are the thicknesses of the 3C and 2H slabs respectively. In practice, the VBO values at the two



(a)



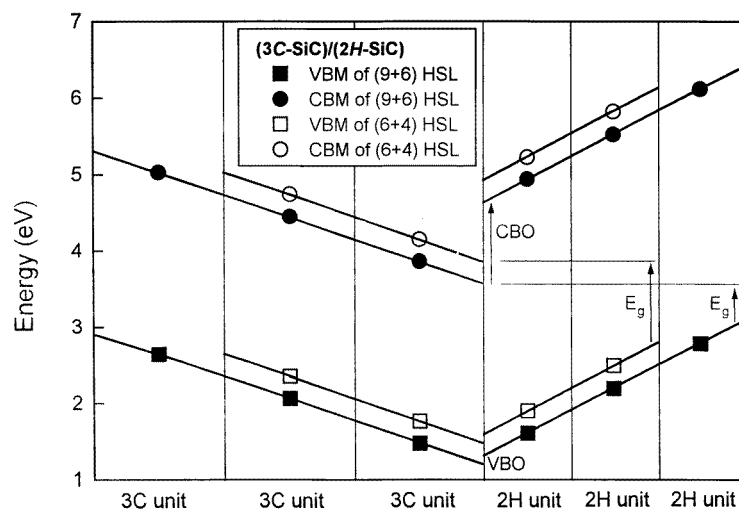
(b)

Figure 2. The line-ups of the VBMs and the CBMs in the 3C slab and in the 2H slab of: (a) (3C-BN)_{3n}/(2H-BN)_{2n}; (b) (3C-GaN)_{3n}/(2H-GaN)_{2n}; (c) (3C-SiC)_{3n}/(2H-SiC)_{2n}, ($n = 2, 3$). The scissors corrections to the LDA band gaps of all constituents are already included.

interfaces may differ slightly from each other, so we use the following relation to calculate the ΔE_g

$$\Delta E_g = -\frac{1}{2}[d(3C) \times \text{IEF}(3C) + d(2H) \times \text{IEF}(2H)]. \quad (2)$$

In table 2 the values of ΔE_g obtained from both the self-consistent calculations and equation (2) are listed. It can be found that the two sets of results are in good agreement with each other. Here, we would like to point out that the present calculations are performed in



(c)

Figure 2. (Continued)

the framework of the ASA and the charge densities of valence electrons in all atomic spheres and empty spheres are spherically symmetrized. In this case the spontaneous polarization in the 2H structures may be overestimated. As a result, the value of the IEF in the SiC HSL given by our calculations (see table 2) is larger than those obtained in [2] (see figure 1 of [2]). However, this factor does not change the conclusions reached here. In fact, for the (3C-SiC)/(2H-SiC) system the value of VBO and the relative distributions of the electric potentials in both the 3C-SiC and 2H-SiC slabs indicated by this work agree well with the results obtained by the *ab initio* pseudopotential calculations in [2].

3.3. Influences of interface relaxation

In the above calculations the relaxations of the interface structures are not taken into account. Since the HSLs studied here are lattice-matched, this effect can be expected to be fairly small. For SiC HSLs Bechstedt and Kackell [3] have performed *ab initio* energy minimization calculations to investigate the atomic relaxations near the interfaces. They found that the strongest atomic relaxations happen in the interfaces between purely cubically and hexagonally stacked layers and the atomic displacements parallel to the *c* axis are negligible inside the material layers. The two Si-C bonds around the interface 3C \rightarrow 2H possess lengths increased by 0.01–0.02 Å, while the bonds in the interface 2H \rightarrow 3C remain almost unchanged. In order to investigate the influence of the atomic relaxations near the interfaces on the present results, we have further calculated the (3C-SiC)_{3n}/(2H-SiC)_{2n} ($n = 1, 2, 3$) with one Si-C bond beside the interface 3C \rightarrow 2H being increased by 0.02 Å. The results are listed in table 2. It appears that the influence of the interface relaxation on the band-gap reduction and the IEF is really small. The maximum change in the band-gap reduction is 0.06 eV, and the value of IEF(2H) – IEF(3C) is almost kept unchanged. On the other hand, the influence of the interface relaxation on the band offset turns out to be remarkable. The interface relaxation considered here only takes place in one of the two nonequivalent interfaces and, as a result, it leads to different band offsets

at the two interfaces (0.16 eV for the unrelaxed interface and 0.26 eV for the relaxed interface). The VBO determined by using the self-consistent potential parameters of the centre 3C bilayer and the centre 2H bilayer is 0.21 eV which is notably larger than the value of 0.14 eV for the unrelaxed structure. The change in the VBO at the relaxed interface can also be estimated by considering the change in the average potentials from one side of a plane of displaced atoms to the other by the following equation

$$\Delta\text{VBO} = (4\pi/A_0)Z^B d/\epsilon_\infty \quad (3)$$

where A_0 is the area of the plane per atom, Z^B is the Born effective charge, d is the displacement and ϵ_∞ the dielectric constant. The values of Z^B and ϵ_∞ given by the calculations of Karch *et al* [12] are $2.81e$ and 7.27 respectively. d is equal to 0.002 \AA in the present case. Using these data we get a value of 0.16 eV for ΔVBO which is in good agreement with the value of 0.12 eV given by the *ab initio* calculation.

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