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Band discontinuity at the (311) *A* GaAs/AlAs interface and possibility of its control by Si insertion layers

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A theoretical analysis of the valence-band discontinuity (ΔE_v) at the high-index (311)*A* GaAs/AlAs interface is reported together with a possibility of ΔE_v control by Si-insertion layers. The calculations are performed by using a self-consistent sp^3s^* tight-binding method in a $(\mathrm{GaAs})_6/(\mathrm{AlAs})_5$ (311) superlattice. The ΔE_v at the (311)*A* interface is calculated to be 0.50 eV, which is practically equal to the ΔE_v of 0.51 eV at the (100) and (110) low-index interfaces. The orientation independence of the ΔE_v holds for the (311)*A* high-index interface. The result of the calculations is consistent with our experimental determination by x-ray photoemission spectroscopy. At the (311)*A* interface, the inserted Si double layers can have two possible layer spacings; one is $a/(4\sqrt{11})$ on As-terminated GaAs and the other $3a/(4\sqrt{11})$ on Ga-terminated GaAs, where a is the lattice constant. In the former case, ΔE_v is calculated to be -0.12 eV (reduced by 0.62 eV), while in the latter it is 1.67 eV (increased by 1.17 eV). ΔE_v depends almost linearly on the Si layer thickness (0–2 ML) on an As-terminated GaAs. The result predicts a possibility of ΔE_v control at the (311)*A* GaAs/AlAs interface.

I. INTRODUCTION

A possibility to artificially control the band discontinuity at a semiconductor interface by inserting thin group-IV-element layers has been a hot issue from both scientific and application points of view.[1–8] Muñoz, Chetty, and Martin[1] and Peressi *et al.*[2] predicted theoretically that the band discontinuity at the (100) GaAs/AlAs interface can be controlled by inserting (Ge_2) or (Si_2) double layers. Sorba *et al.*[3] observed shifts in the core levels of x-ray photoemission spectroscopy (XPS) from the (100) GaAs/AlAs interface with the Si insertion layers and attributed the shifts to the success of band discontinuity control. However, Hashimoto and coworkers[4–6] and Akazawa *et al.*[7] have shown that the inserted Si atoms mainly act as donors and do not serve to control the band discontinuity because no Si-induced interface dipole is formed.[4–7] The occupation-site control of Si atoms at the (100) interface is crucial in forming an interface dipole to control the band discontinuity.[4–6]

On the other hand, it has been shown experimentally that, on a (311) *A* GaAs substrate, doped Si can be either an acceptor or a donor depending on growth conditions.[9–11] This indicates that we have a higher possibility to successfully form a Si-induced interface dipole and control the band discontinuity at the (311)*A* GaAs/AlAs interface. However, theoretical calculations on the band discontinuity and a possibility to control it have not been reported for the (311)*A* GaAs/AlAs interface, which is grown on a high-index surface.

The purpose of this paper is to clarify theoretically (1) how large the valence-band discontinuity (ΔE_v) is at the (311)*A* GaAs/AlAs interface and (2) how much the ΔE_v can be controlled by insertion of Si double-layers at the interface.

The calculations are performed by using a self-consistent tight-binding method[12,13] as described in Sec. II. The result of (1) is shown and compared with our experimental ΔE_v measured by the XPS in Sec. III. We discuss whether the orientation independence of ΔE_v holds for the high-index (311)*A* interface. The result of (2) is shown in Sec. IV. Our preliminary results for the (100) and (110) low-index interfaces were reported in Ref. 5.

II. METHOD OF CALCULATIONS

The calculations are performed on the basis of the sp^3s^* semiempirical tight-binding method.[14] The method for the self-consistent calculation of ΔE_v is essentially the same as that of Muñoz and co-workers.[12,13,15] We describe the method briefly as follows.

First, we begin with the situation that GaAs and AlAs are separated. We adopt the tight-binding parameters of bulk GaAs and AlAs from the values of Vogl, Hjalmarson, and Dow[14] which reproduce band structures of individual semiconductors accurately.[14] In our study, the spin-orbit coupling is not included. Additionally we need to assume a "natural" valence-band discontinuity ΔE_v^0, which is defined as a valence-band discontinuity when the two semiconductors are separated,[16] i.e., there is no difference between the average potentials in both semiconductors. We assume $\Delta E_v^0=0.24$ eV and shift the atomic-orbital energies of AlAs by this value relative to those of GaAs. This value is obtained by equalizing the mean sp^3 energies of both semiconductors as done by Muñoz, Sánchez-Dehesa, and Flores.[12]

Second, we model the formation of the (311)*A* GaAs/AlAs interface by a (311) GaAs/AlAs superlattice (SL) and calculate ΔE_v. As an initial condition, we start with a zero dipole across the interface, i.e., no difference in the average potentials in GaAs and AlAs. To do so,

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we keep the above atomic-orbital energies. Based on the initial Hamiltonian, (1) we calculate charges on the atoms, (2) obtain charge densities per area on the atomic planes parallel to the interface, (3) solve the Poisson's equation under the periodic boundary condition of the SL to get changes in the potentials on the atomic planes due to charge redistributions at the interface, and (4) modify the initial atomic-orbital energies according to the changes in the potentials. The process (1)–(4) is iterated until the self-consistency is achieved. Consequently, ΔE_v is obtained as $\Delta E_v = \Delta E_v^0 + \Delta V$, where ΔV is the dipole defined as the difference between the average potentials in GaAs and AlAs.

One difference between our method and that of Muñoz and co-workers[12,13,15] is that we apply the method to SL's while they applied their method to heterojunctions between two semi-infinite semiconductors. In addition, we allow modifications of atomic-orbital energies on all atomic planes in a SL, while they did within a limited number of atomic planes (four or five) (Refs. 12, 13, 15) around an interface. Better accuracy is expected in our calculation. We showed preliminary calculations by using the same method for the (100) and (110) GaAs/AlAs interfaces in Refs. 5 and 8.

Last, we insert Si double layers at the (311)*A* GaAs/AlAs interface. We assume that the inserted Si atoms occupy lattice sites of ideal zinc-blende structure. The Si lattice ($d = 2.35$ Å) is hydrostatically deformed to match the GaAs and AlAs lattices ($d = 2.45$ Å), where d is the bond length. The interatomic tight-binding parameters of Si are assumed to be proportional to $d^{-\eta_{\alpha,\beta}}$, where α and β ($=s$, p_x, p_y, p_z, and s^*) are the adjacent orbitals. We adopt the exponents $\eta_{\alpha,\beta}$ from the values of Hong *et al.*[18] The effect of lattice relaxation was proved to be unimportant at the (100) and (110) GaAs/AlAs interfaces.[2,17]

In the actual calculations, we use a $(\mathrm{GaAs})_6/(\mathrm{AlAs})_5$ (311) SL. Its primitive translation vectors are

$$\mathbf{a}_1 = \frac{a}{2}[\sqrt{2}\mathbf{x}] , \quad \mathbf{a}_2 = \frac{a}{2}\left[\frac{1}{\sqrt{2}}\mathbf{x} + \sqrt{11/2}\mathbf{y} \right] ,$$
$$\mathbf{a}_3 = \frac{a}{2}[2\sqrt{11}\mathbf{z}] . \tag{1}$$

Here **x**, **y**, and **z** are the Cartesian unit vectors defined for the SL, which are oriented along the $[0\bar{1}1]$, $[2\bar{3}\bar{3}]$, and [311] directions, respectively. a is the lattice constant of GaAs. The vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ are on the (311) plane, and $\mathbf{a}_3$ is along the [311] direction. In general, $\mathbf{a}_3$ of the $(\mathrm{GaAs})_m/(\mathrm{AlAs})_n$ (311) SL takes the [311] direction when $m+n = (\text{integer}) \times 11$, hence we choose $m = 6$ and $n = 5$. In this SL, the atomic planes are stacked in the sequence:

$$\cdots \text{—Al-As—Al-}\overset{(B)}{\text{As}}\text{—Ga-As—Ga-As—} \cdots \text{—Ga-As—Ga-}\overset{(A)}{\text{As}}\text{—Al-As—Al-As—} \cdots ,$$

where the spacing between two planes is $a/(4\sqrt{11})$ for Ga-As and Al-As pairs, and $3a/(4\sqrt{11})$ for As—Ga and As—Al pairs. (*A*) and (*B*) denote the (311)*A* and (311)*B* GaAs/AlAs interfaces, which are originally the As-terminated (311)*A* and (311)*B* GaAs surfaces, respectively. We focus mainly on the (311)*A* interface, which is formed by AlAs growth on a (311)*A* GaAs substrate.

III. BAND DISCONTINUITY AT THE (311) *A* GaAs/AlAs INTERFACE

Figure 1 shows the atomic arrangement (a) and the potential profile (b) at the (311)*A* GaAs/AlAs interface. We assume that the interface is flat, having neither facets nor interdiffusion across the interface. The potential oscillates sawtoothlike due to the negative and positive charges on the anions and cations, respectively.[8,13] The average potentials in GaAs and AlAs are calculated from the potentials on a few central planes of respective semiconductors, excluding potentials that change transiently at the interface. As the difference between the average potentials, we obtain $\Delta V = 0.26$ eV. Finally, ΔE_v at the (311)*A* interface is calculated to be 0.50 eV, i.e., $\Delta E_v = \Delta E_v^0 + \Delta V = 0.24\ \text{eV} + 0.26\ \text{eV}$. At the same time, we obtain $\Delta V = 0.28$ eV and hence $\Delta E_v = 0.52$ eV at the (311)*B* interface.

For comparison, Fig. 2 shows the potential profiles at the (100) and (110) GaAs/AlAs low-index interfaces. The interface formations are modeled by (100) and (110) $(\mathrm{GaAs})_6/(\mathrm{AlAs})_6$ SL's. The differences in amplitude of the potential oscillation reflect the difference in interface orientations. However, we obtain $\Delta V = 0.27$ eV and hence $\Delta E_v = 0.51$ eV at both interfaces. Our results of ΔE_v at the high- and low-index interfaces are summarized in Table I together with ΔE_v at low-index interfaces calculated by Muñoz, Sánchez-Dehesa, and Flores.[15] From these calculations, it is found that ΔE_v at a GaAs/AlAs interface is almost constant for various interface orientations, *even for a high-index interface.*

In experiments, Hirakawa, Hashimoto, and Ikoma[19] showed the orientation independence of ΔE_v at a GaAs/AlAs interface *only for low-index interfaces;* (100), (110), and (111)*B*. ΔE_v was measured by the *in situ* XPS for the samples grown by molecular beam epitaxy (MBE).[19] In the present paper, we carried out XPS measurements of ΔE_v at the *high-index* (311)*A* (and *B*) interface to confirm our theoretical calculations. The samples were grown on (311)*A* n^+-GaAs substrates: (1) AlAs(30 Å)/GaAs(1 μm)/GaAs(substrate) for the (311)*A* interface, and (2) GaAs(30 Å)/AlAs(100 Å)/GaAs(1 μm)/GaAs(substrate) for the (311)*B* interface. The growth temperature was 600 °C for all the layers. For both samples, we measured ΔE_v at the interface between the two layers indicated by the underlines. In the latter sample, the top GaAs(30 Å) layer is grown on the (311)*A* surface of the AlAs(100 Å) layer. This is equivalent to the interface formation where an AlAs layer is grown on a (311)B surface of GaAs. The XPS measurements were carried out with an Al $K\alpha$ monochromatic x-ray source of $h\nu = 1486.6$ eV. ΔE_v is determined by using an energy difference between the Ga 3d and Al 2p core levels. The details of the measurement technique are described in Ref. 19. ΔE_v's measured in the present study and Ref. 19 are included in Table I. In the experiments, ΔE_v is found to be independent of the interface orientation even at the high-index (311)A (and B) interface, which confirms our calculations.

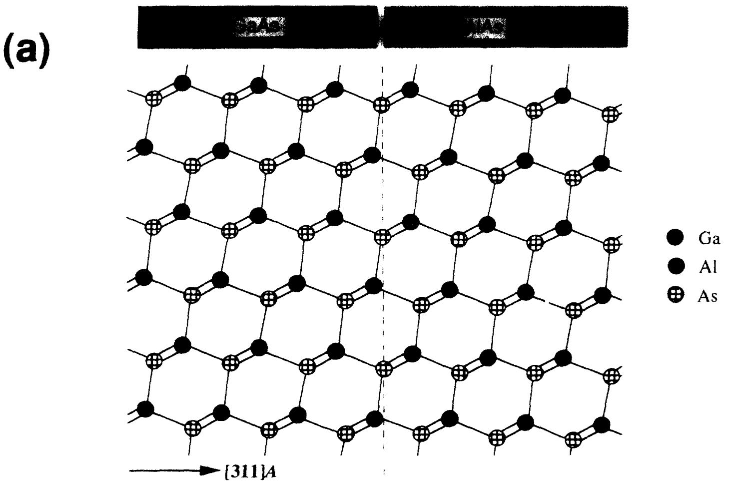
IV. EFFECTS OF Si-INSERTION LAYERS ON BAND DISCONTINUITY

We insert Si double layers at the (311)A interface in a $(\mathrm{GaAs})_6/(\mathrm{AlAs})_5$ (311) SL. The Si double layers can have two possible configurations,

$$\cdots\text{—Al-As—}\overset{(B)}{\text{Al-As}}\text{—Ga-As—Ga-As—}\cdots\text{—Ga-}\overset{(A)}{\text{As}}\text{—Si-Si—Al-As—Al-As—}\cdots\,,$$

$$\cdots\text{—Al-As—}\overset{(B)}{\text{Al-As}}\text{—Ga-As—Ga-As—}\cdots\text{—Ga-}\overset{(A)}{\text{Si}}\text{—Si-As—Al-As—Al-As—}\cdots\,.$$

The former is formed on an As-terminated GaAs; the first Si plane occupies Ga sites and the second occupies As sites with the interplanar spacing of $a/(4\sqrt{11})$. The latter is formed on a Ga-terminated GaAs; the occupation sites are reversed and the interplanar spacing is $3a/(4\sqrt{11})$. Here the inserted Si atoms are assumed to occupy lattice sites of the ideal zinc-blende structure as mentioned in Sec. II. We insert no Si layers at the (311)B interface. Figures 3(a) and 3(b) show the atomic arrangements at the (311)A interface with the Si double layers on an As-terminated and a Ga-terminated GaAs, respectively. From the viewpoint of chemical valence, we can re-



(311)A interface

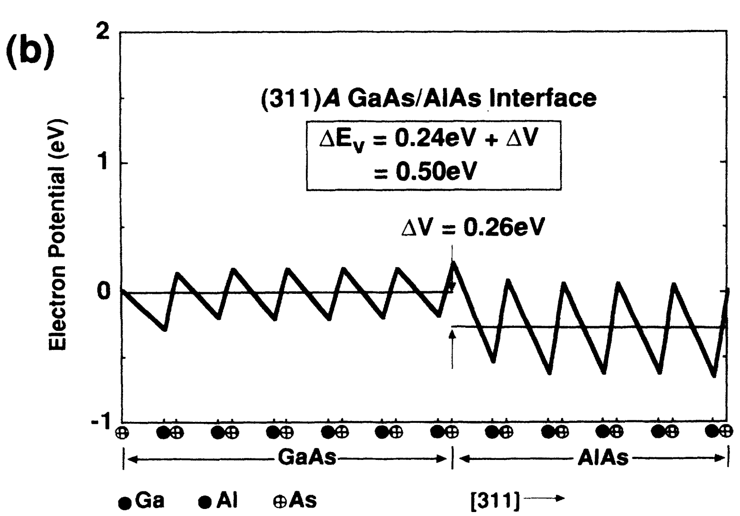


FIG. 1. Atomic arrangement (a) and potential profile (b) at the high-index (311)A GaAs/AlAs interface. The vertical dashed line in (a) indicates the interface. The average potentials in GaAs and AlAs are indicated by thin solid lines in (b).

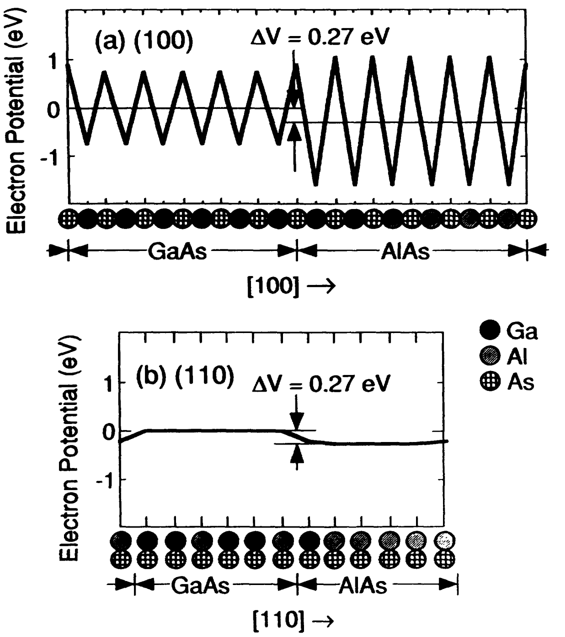


FIG. 2. Potential profiles at GaAs/AlAs low-index interfaces: (a) (100) and (b) (110) interfaces.

TABLE I. Valence-band discontinuities ΔE_v (in eV) at GaAs/AlAs interfaces.

Interface	Theory This study	 Muñoz *et al.*[a]	Experiment
(311)*A*	0.50		0.42,0.44
(311)*B*	0.52		0.45
(100)	0.51	0.38	0.44 ± 0.05[b]
(110)	0.51	0.32	0.44 ± 0.05[b]

[a] Reference 15.

[b] Reference 19.

gard the Si double layers as consisting of a positively charged donorlike plane (Ga site) and a negatively charged acceptorlike plane (As site) and acting as a microscopic capacitor[1,2] to control ΔE_v.

Figures 4(a) and 4(b) show the potential profiles at the (311)*A* GaAs/AlAs interface with the Si double layers on an As-terminated and a Ga-terminated GaAs, respectively. ΔV is -0.36 eV in the former and 1.43 eV in the latter. The change of ΔV from the original value is -0.62 eV and $+1.17$ eV, respectively. By using the relation $\Delta E_v = \Delta E_v^0 + \Delta V$ with $\Delta E_v^0 = 0.24$ eV as shown in Sec. II, ΔE_v with the Si double layers is deduced as $\Delta E_v = -0.12$ eV on an As-terminated GaAs, and $\Delta E_v = 1.67$ eV on a Ga-terminated GaAs. The sign of the ΔE_v change depends on the polarity of the terminated plane of GaAs and the magnitude mainly on the interplanar spacing of the Si double layers. The gradient of the average potentials in GaAs and AlAs in Fig. 4 is an artifact caused by the periodic boundary condition of the SL as shown in Refs. 1 and 8. This does not influence the results of ΔE_v calculations.

In the previous work,[5] we studied the effects of Si insertion layers at the (100) and (110) low-index interfaces. With Si double layers, ΔE_v is calculated to be -1.36 and 2.1 eV at the As- and Ga-terminated (100) interfaces, respectively, and 0.35 eV at the (110) interface. It should be noted that an effect of the Si insertion layers on ΔE_v has a strong orientation dependence, although ΔE_v with no Si layers is independent of the interface orientation.

To calculate ΔE_v at a GaAs/AlAs interface as a function of the inserted Si layer thickness, $d(0\sim 2$ ML), for various interface orientations, we insert Si atoms as follows. (1) At the (311)*A* interface with an As-terminated GaAs, the Si atoms are inserted as

$$\cdots\text{—Ga-}\overset{(A)}{\text{As}}\text{—}(\mathbf{Si}_{d/2}\text{Ga}_{1-d/2})-(\mathbf{Si}_{d/2}\text{As}_{1-d/2})\text{—Al-As—Al-As—}\cdots .$$

(2) At the (100) interface, the Si atoms are inserted as

$$\cdots\text{—Ga—As—}(\mathbf{Si}_{d/2}\text{Ga}_{1-d/2})-(\mathbf{Si}_{d/2}\text{As}_{1-d/2})\text{—Al—As—}\cdots$$

and

$$\cdots\text{—As—Ga—}(\mathbf{Si}_{d/2}\text{As}_{1-d/2})-(\mathbf{Si}_{d/2}\text{Ga}_{1-d/2})\text{—As—Al—}\cdots ,$$

for As- and Ga-terminated GaAs, respectively, where the interplanar spacing is $a/4$. (3) At the (110) interface, the Si atoms with $0\le d\le 1$ are inserted as

$$\cdots-\begin{bmatrix}\text{Ga}\\ \text{As}\end{bmatrix}-\begin{bmatrix}(\mathbf{Si}_d\text{Ga}_{1-d})\\ (\mathbf{Si}_d\text{As}_{1-d})\end{bmatrix}-\begin{bmatrix}\text{Al}\\ \text{As}\end{bmatrix}-\cdots ,$$

where the interplanar spacing is $a/(2\sqrt{2})$. With $1\le d\le 2$,

$$\cdots-\begin{bmatrix}\text{Ga}\\ \text{As}\end{bmatrix}-\begin{bmatrix}\mathbf{Si}\\ \mathbf{Si}\end{bmatrix}-\begin{bmatrix}(\mathbf{Si}_{d'}\text{Ga}_{1-d'})\\ (\mathbf{Si}_{d'}\text{As}_{1-d'})\end{bmatrix}-\begin{bmatrix}\text{Al}\\ \text{As}\end{bmatrix}-\cdots ,$$

where $d' = d-1$. We assume that the Si atoms occupy Ga and As sites with the equal probabilities for any d.

The number of the inserted Si atoms per unit area N_{Si} is expressed as

$$N_{\text{Si}} = dN_a . \tag{2}$$

Here N_a is the number of atomic sites per unit area on the atomic plane,

$$N_a = 4/(a^2\sqrt{11}),\ 2/a^2,\ \text{and}\ 2\sqrt{2}/a^2\ , \tag{3}$$

for (311)A, (100), and (110) interfaces, respectively. The relation among ds for the different interface orientations, denoted as d^{311A}, d^{100}, and d^{110}, which gives the equal N_{Si} is

$$d^{100} = (2/\sqrt{11})d^{311A} = \sqrt{2}d^{110}\ . \tag{4}$$

This relation is used to compare ΔE_v in Fig. 5.

Figure 5 shows ΔE_v at GaAs/AlAs interfaces as a function of d obtained by the present calculations. The horizontal axis indicates d for the (100) interface, d^{100}, which is related to d^{311A} and d^{110} as mentioned above. ΔE_v changes almost linearly with increasing d and the amount of change depends strongly on the interface orientations. The theoretical line for the As-terminated (311)A interface, which is the main concern of this study, lies between those for the (110) and As-terminated (100) interfaces.

In Fig. 5, we also plot the average valence-band difference $\Delta\tilde{E}_v$ measured for the various interface orientations by Hashimoto *et al.*[4-6] and the (100) interface by Sorba *et al.*[3] $\Delta\tilde{E}_v$ is defined as[4-6]

$$\Delta\tilde{E}_v = \Delta E_{\mathrm{CL}}\ (\text{measured}) + E_{v\text{-Ga }3d} - E_{v\text{-Al }2p}\ . \tag{5}$$

Here ΔE_{CL} (measured) is the measured energy separation between Ga 3d and Al 2p peaks in the XPS which depends on both a band bending and a true change in ΔE_v. $E_{v\text{-Ga 3d}}$ and $E_{v\text{-Al }2p}$ denote the binding energies of Ga 3d and Al 2p core levels measured from the valence-band maxima in GaAs and AlAs, respectively. As shown in Fig. 5, $\Delta\tilde{E}_v$ does not exhibit orientation nor thickness dependences as expected from the present calculations of ΔE_v, where the Si insertion layers change ΔE_v. On the other hand, the change in $\Delta\tilde{E}_v$ is in good agreement with the theoretical line assuming a band bending in the AlAs overgrown layer, where the inserted Si atoms mainly act as donors, as already shown by Hashimoto, Tanaka, and Ikoma (Fig. 3 in Ref. 6). The present study further confirms the conclusion of Hashimoto and co-workers[4-6] that the role of the Si insertion layers is not a control of ΔE_v as proposed by Sorba *et al.*[3] but an introduction of band bending.

To achieve a true control of ΔE_v by the Si insertion layers, the occupation-site control of Si atoms is crucial. Recently, Agawa *et al.*[11] found that δ-doped Si atoms act

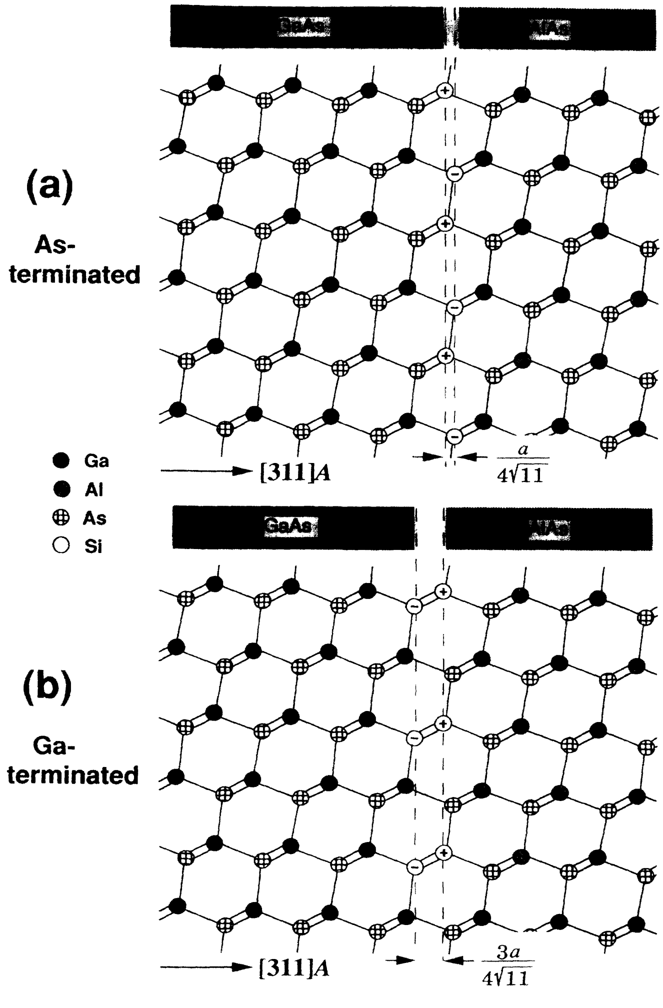


FIG. 3. Atomic arrangements at the high-index (311)A GaAs/AlAs interface inserted with the Si double layers. GaAs is (a) As-terminated and (b) Ga-terminated. The Si double layers consist of a donorlike plane and an acceptorlike plane, indicated by "+" and "−", respectively.

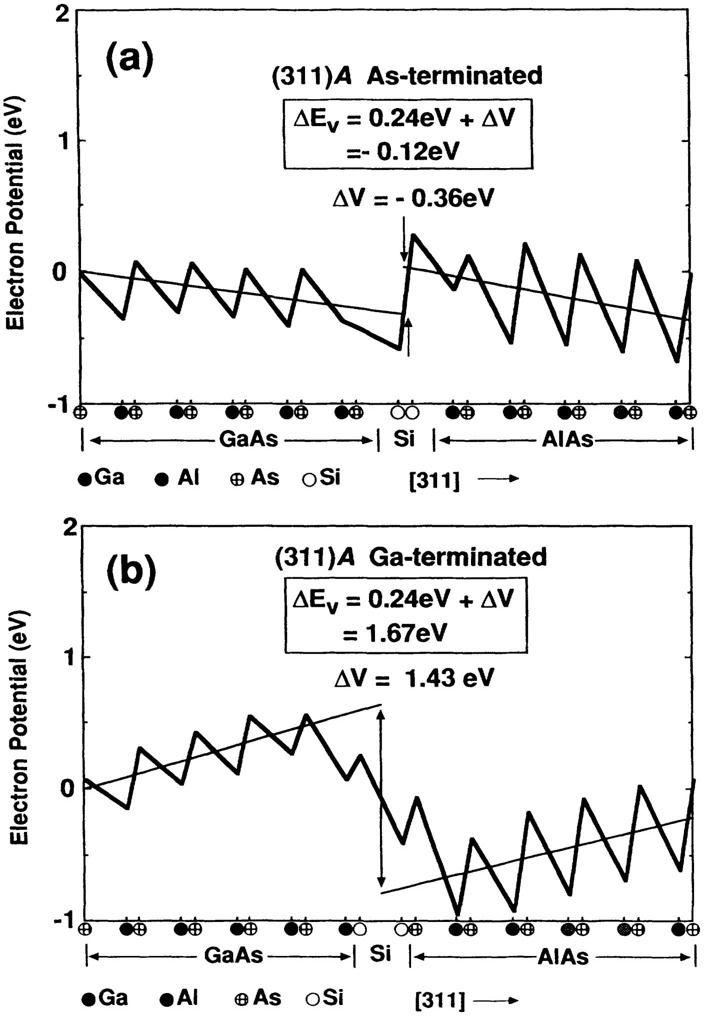


FIG. 4. Potential profiles at the high-index (311)*A* GaAs/AlAs interface inserted with the Si double layers. GaAs is (a) As-terminated and (b) Ga-terminated.

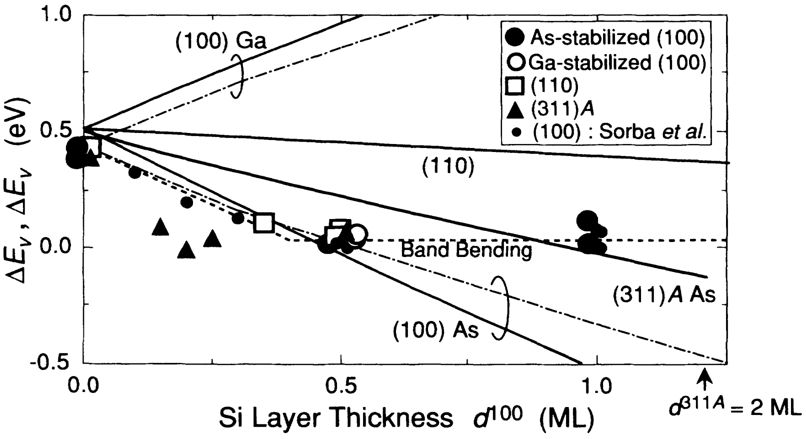


FIG. 5. Valence-band discontinuities ΔE_v at GaAs/AlAs interfaces as a function of the inserted Si layer thickness d. The horizontal axis indicates d for the (100) interface, d^{100}. The solid lines indicate ΔE_v calculated in the present study for the (311)*A* As, (100)As, (100)Ga, and (110) interfaces, where As and Ga indicate As- and Ga-terminated GaAs, respectively. The dash-dot lines indicate ΔE_v calculated by Peressi *et al.* (Ref. 2) for the (100)As and (100)Ga interfaces. The symbols (●, ○, □, and ▲) indicate the average valence-band difference $\Delta \tilde{E}_v$ measured for As- and Ga-stabilized (100), (110), and (311)*A* interfaces, respectively, by Hashimoto and co-workers (Refs. 4–6). The symbol (•) indicates $\Delta \tilde{E}_v$ measured for the As-stabilized (100) interface by Sorba *et al.* (Ref. 3). The dashed line shows the theoretical $\Delta \tilde{E}_v$ obtained by assuming a band bending in the AlAs overgrown layer by Hashimoto and co-workers (Refs. 4–6).

as donors and acceptors on a (311)A GaAs substrate when the growth temperature is lower and higher than a critical temperature of 480 °C, respectively. This suggests that the (311)A interface is more promising to control ΔE_v because the Si sites can be controlled by changing a growth temperature of MBE.

In the present calculation, we assume that the (311)A (and B) interface is atomically flat. In experiments, Nötzel *et al.*[20] reported a periodic corrugation of the (311)A interface grown by MBE. They described the (311)A GaAs surface by (311) terraces and two sets of {331} facets based on the analysis of reflection high-energy electron-diffraction patterns.[20] To predict the effects of Si insertion layers at the corrugated interface, it is necessary to study their effects at the {331} facets. This may require further theoretical investigation, which is beyond the present study.

V. CONCLUSIONS

We analyzed ΔE_v at the (311)A GaAs/AlAs interface and a possibility of ΔE_v control by insertion of the Si double layers by using the self-consistent tight-binding method. The results are summarized as follows.

(1) ΔE_v at the (311)A (and B) high-index interface is calculated to be 0.50 eV (and 0.52 eV), which is practically equal to ΔE_v of 0.51 eV at the (100) and (110) low-index interfaces. The orientation independence of ΔE_v holds for the (311)A (and B) high-index interface, being consistent with our experimental observation by the XPS.

(2) With insertion of Si double layers, ΔE_v at the (311)A interface is calculated to be −0.12 eV (reduced by 0.62 eV) and 1.67 eV (increased by 1.17 eV) on an As-terminated and a Ga-terminated GaAs, respectively. ΔE_v depends almost linearly on the Si layer thickness (0–2 ML) on an As-terminated GaAs. The result predicts a possibility to control ΔE_v at the (311)A GaAs/AlAs interface.

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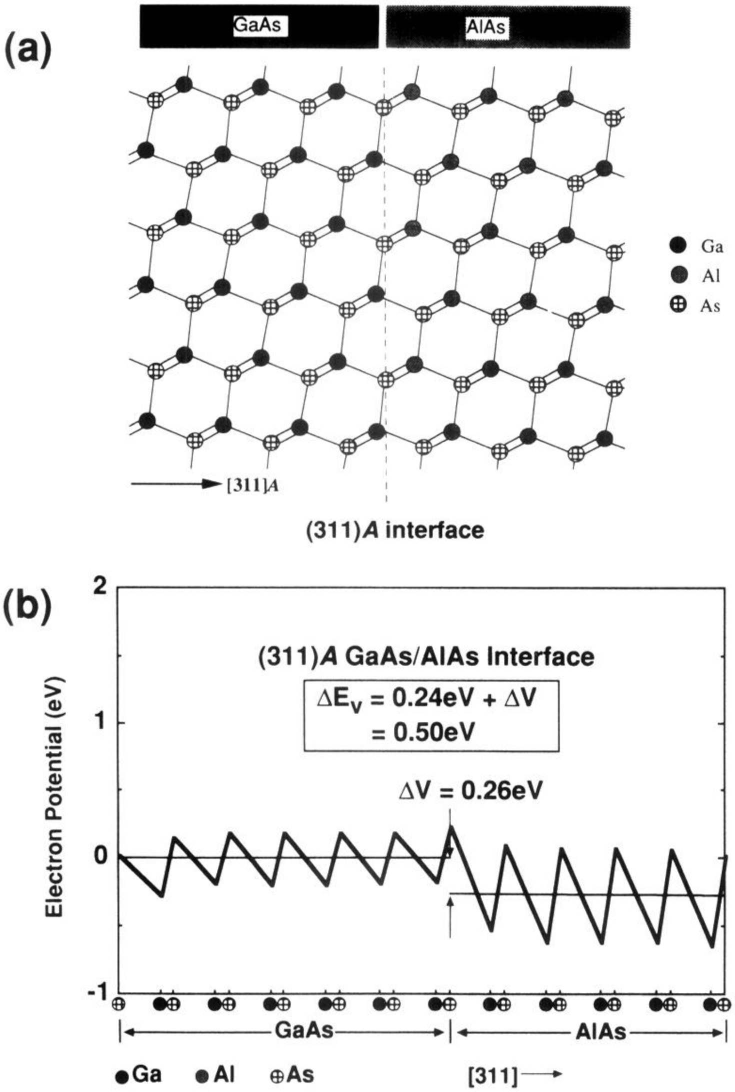

FIG. 1. Atomic arrangement (a) and potential profile (b) at the high-index (311)*A* GaAs/AlAs interface. The vertical dashed line in (a) indicates the interface. The average potentials in GaAs and AlAs are indicated by thin solid lines in (b).

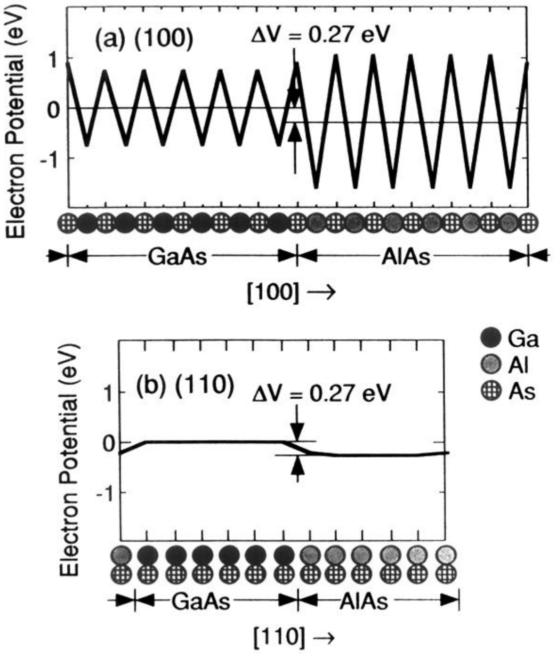

FIG. 2. Potential profiles at GaAs/AlAs low-index interfaces: (a) (100) and (b) (110) interfaces.

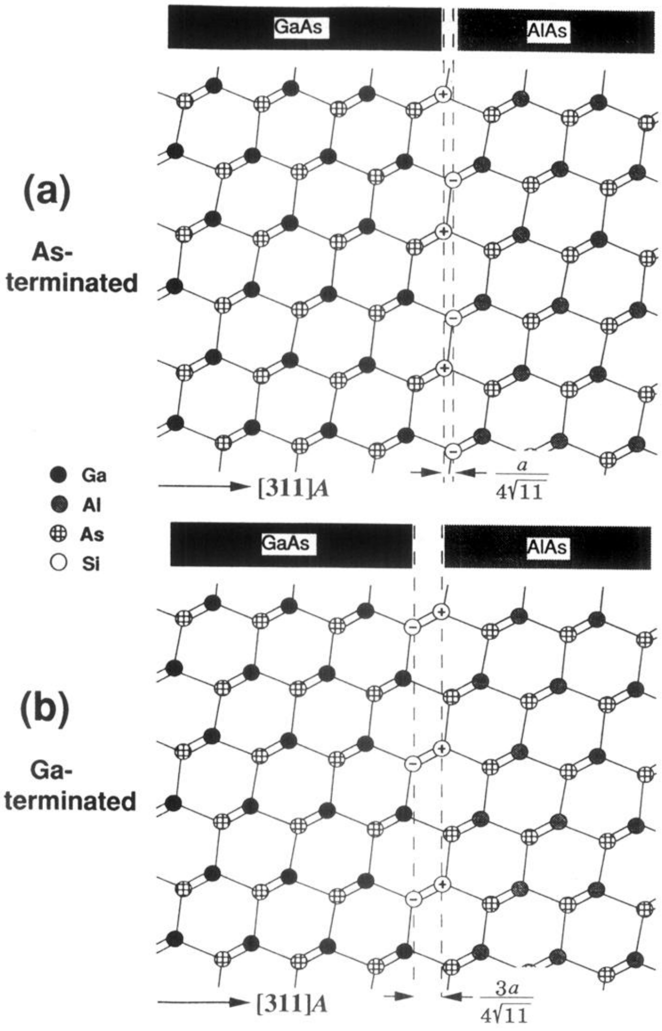

FIG. 3. Atomic arrangements at the high-index (311)*A* GaAs/AlAs interface inserted with the Si double layers. GaAs is (a) As-terminated and (b) Ga-terminated. The Si double layers consist of a donorlike plane and an acceptorlike plane, indicated by "+" and "−", respectively.