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Possibility of Band-Discontinuity Control at (100) GaAs/AlAs Interfaces by ZnSe Insertion Layers

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We have theoretically analyzed the valence-band discontinuity (ΔE_v) at the (100) GaAs/AlAs interfaces with the $(ZnSe)_x$ insertion layers ($0 \leq x \leq 0.5$). The theoretical calculation is carried out by the self-consistent sp^3s^* tight-binding method. The $(ZnSe)_x$ layer is inserted as; –Ga–As–[$\mathbf{Zn}_x\mathrm{Ga}_{1-x}$]–[$\mathbf{Se}_x\mathrm{As}_{1-x}$]–Al–As– and –As–Ga–[$\mathbf{Se}_x\mathrm{As}_{1-x}$]–[$\mathbf{Zn}_x\mathrm{Ga}_{1-x}$]–As–Al–, for the As-terminated and the Ga-terminated GaAs, respectively. With the $(ZnSe)_{0.5}$ insertion layer, ΔE_v is calculated to be 1.70 eV (As-terminated GaAs) and −0.82 eV (Ga-terminated GaAs), which are larger by 1.19 eV and smaller by 1.33 eV, respectively, than $\Delta E_v = 0.51$ eV (no insertion layers). The magnitude of the change due to the $(ZnSe)_x$ layer is slightly larger than that due to the $(Si_2)_x$ layer.

1. INTRODUCTION

The band discontinuities at the (100) GaAs/AlAs interfaces with impurity insertion layers have been analyzed theoretically and experimentally in order to understand and control the interfaces [1–5]. The insertion of the Si(group IV) double-layers at the interface [–Ga–As–**Si**–**Si**–Al–As–] controls the band discontinuity as shown by the theoretical calculations [2, 3]. The change in the band discontinuity is caused by the dipole of the **Si**(donor-site)–**Si**(acceptor-site) pair. On the other hand, the insertion of the In(group III) monolayer [–Ga–As–**In**–As–Al–As–] does not change the band discontinuity [4], and that of the P(group V) monolayer [–Ga–As–Ga–**P**–Al–As–] changes it very slightly [5]. Isoelectronic impurities, such as In and P, do not have a doping effect which can change the band discontinuity largely.

In contrast with the above, effects of the ZnSe(group II-VI) insertion layers have not been studied in spite of the fact that the growth of ZnSe on GaAs is possible in the present growth technology. The insertion of the ZnSe layer [–Ga–As–**Zn**–**Se**–Al–As–] can induce the dipole of the **Zn**(acceptor-site)–**Se**(donor-site) pair, indicating a possibility of the change in the band discontinuity.

In this study, we theoretically analyze the valence-band discontinuity (ΔE_v) at the (100) GaAs/AlAs interface with the $(ZnSe)_x$ insertion layers ($0 \leq x \leq 0.5$) to clarify how large the insertion layers can change ΔE_v. The theoretical calculation of ΔE_v is carried out by the self-consistent sp^3s^* tight-binding method [3, 6]. To obtain ΔE_v, we calculate the potential profile and the dipole at the interfaces.

2. METHOD OF CALCULATION

The calculation of ΔE_v is carried out by using the self-consistent tight-binding method [3, 6] with the sp^3s^* basis [7]. In this method, the atomic orbital energies are modified repeatedly according to the changes in the electrostatic potentials induced on the atomic planes, as proposed by Muñoz *et al.* [6] The tight-binding parameters are taken from the values of Vogl *et al.* [7] The spin-orbit coupling is not included.

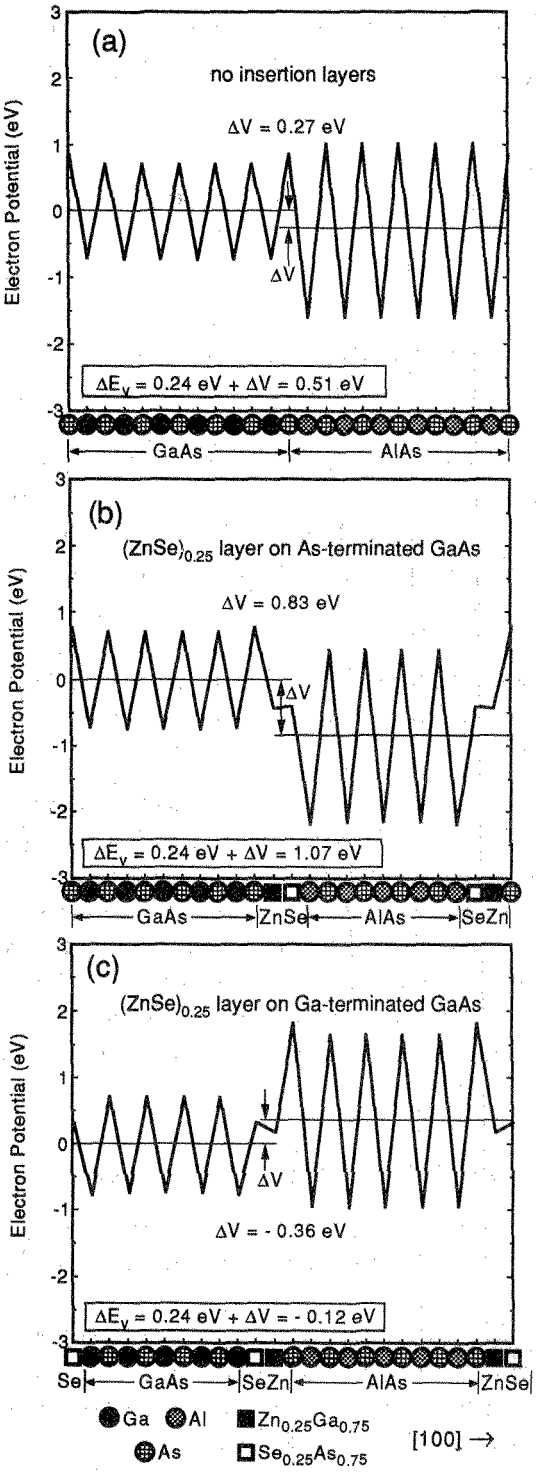

Figure 1: Potential profiles at the (100) GaAs/AlAs interfaces with: (a) no insertion layers, (b) the $(ZnSe)_{0.25}$ layer on As-terminated, and (c) the $(ZnSe)_{0.25}$ layer on Ga-terminated GaAs.

The $(GaAs)_6/(AlAs)_6$ [100] superlattice is used as a model of the (100) GaAs/AlAs interface. A lattice strain due to the $(ZnSe)_x$ insertion is neglected, because ZnSe is nearly lattice-matched to GaAs. The details of the method of calculation using the superlattice are described in Ref. [3].

In Ref. [3], we calculated ΔE_v at the (100) GaAs/AlAs interface with no insertion layers by using the above method. Figure 1(a) shows the potential profile at the interface with no insertion layers (adapted from Fig. 2(a) in Ref. [3]). Since the anion- and cation-planes are stacked in turn along the [100] direction, the potential oscillates sawtooth-likely. The dipole (ΔV), which is defined as the difference between the average potential in GaAs and that in AlAs, is 0.27 eV. ΔE_v is obtained as [3];

$$\Delta E_v = \Delta E_v{}^0 + \Delta V. \qquad (1)$$

Here, $\Delta E_v{}^0$ (= 0.24 eV) is the "natural" valence-band discontinuity [8], which is defined as the valence-band discontinuity when the two semiconductors are separated (i.e., $\Delta V = 0$). From Eq. (1), ΔE_v at the (100) GaAs/AlAs interface with no insertion layers is calculated to be 0.51 eV [3]. If the $(ZnSe)_x$ insertion layer changes ΔV, it changes ΔE_v according to Eq. (1).

3. RESULTS AND DISCUSSIONS

We calculate ΔE_v at the (100) GaAs/AlAs interface with the $(ZnSe)_x$ insertion layers with the thickness $0 \leq x \leq 0.5$ ML, because most of the experiments on ΔE_v with insertion layers were carried out in such thickness range [1,3]. We assume that the $(ZnSe)_x$ layer is inserted as;

–Ga–As–[$\mathbf{Zn}_x$Ga$_{1-x}$]–[$\mathbf{Se}_x$As$_{1-x}$] –Al–As–

and

–As–Ga–[$\mathbf{Se}_x$As$_{1-x}$]–[$\mathbf{Zn}_x$Ga$_{1-x}$] –As–Al–,

on the As-terminated and the Ga-terminated GaAs, respectively. Due to the presence of the negatively charged Zn(acceptor-site) and the positively charged Se(donor-site), the dipoles

of the $[\mathbf{Zn}_x\mathrm{Ga}_{1-x}]$-$[\mathbf{Se}_x\mathrm{As}_{1-x}]$ pair and the $[\mathbf{Se}_x\mathrm{As}_{1-x}]$-$[\mathbf{Zn}_x\mathrm{Ga}_{1-x}]$ pair can be induced on the As-terminated and the Ga-terminated GaAs, respectively. Since the polarity of the dipole on the As-terminated GaAs is opposite to that on the Ga-terminated GaAs, the opposite effect to ΔE_v is expected between the two.

Figures 1(b) and 1(c) show the potential profiles at the (100) GaAs/AlAs interfaces with the $(\mathrm{ZnSe})_{0.25}$ insertion layer on the As-terminated and the Ga-terminated GaAs, respectively. The dipole ΔV is 0.83 eV (As-terminated) and -0.36 eV (Ga-terminated). Using Eq. (1), ΔE_v is calculated to be 1.07 eV (As-terminated) and -0.12 eV (Ga-terminated), while $\Delta E_v = 0.51$ eV [3] at the interface with no insertion layers. The insertion of the ZnSe layer changes ΔE_v significantly even with $x = 0.25$ ML.

Figure 2 shows ΔE_v and ΔV at the (100) GaAs/AlAs interfaces with the $(\mathrm{ZnSe})_x$ insertion layer ($0 \leq x \leq 0.5$). As shown in the figure, the sign of the ΔE_v change due to the $(\mathrm{ZnSe})_x$ insertion depends on the polarity of the terminated plane of GaAs and the magnitude of the change depends on the thickness x, clearly showing that the ZnSe-induced dipole controls ΔE_v. For $x = 0.5$ (the maximum x in the present study), we obtain $\Delta E_v = 1.70$ eV (As-terminated) and -0.82 eV (Ga-terminated), which are larger by 1.19 eV and smaller by 1.33 eV, respectively, than $\Delta E_v = 0.51$ eV (no insertion layers). The present result predicts a possibility of the artificial control of ΔE_v at the (100) GaAs/AlAs interface by the insertion of the $(\mathrm{ZnSe})_x$ layer.

In Fig. 2, we also show ΔE_v and ΔV at the (100) GaAs/AlAs interfaces with the $(\mathrm{Si}_2)_x$ insertion layer obtained in our previous study. (See Fig. 5 in Ref. [3]) The magnitude of the ΔE_v change due to the $(\mathrm{ZnSe})_x$ insertion layer is slightly larger than that due to the $(\mathrm{Si}_2)_x$ insertion layer.

To achieve an artificial control of ΔE_v experimentally, the site-control of inserted impurity atoms to form a dipole is crucial. For the Si insertion layers, it is difficult to control the Si-sites and form the **Si**(donor-site)–**Si**(acceptor-site) dipole, because the Si atoms tend to occupy donor-sites on the (100) GaAs [3]. On the other hand, for the ZnSe insertion layers, the site-control to form the **Zn**(acceptor-site)–**Se**(donor-site) dipole is considered to be easier, because the Zn and the Se atoms prefer to occupy acceptor-sites and donor-sites, respectively. The ZnSe insertion is promising to control ΔE_v artificially.

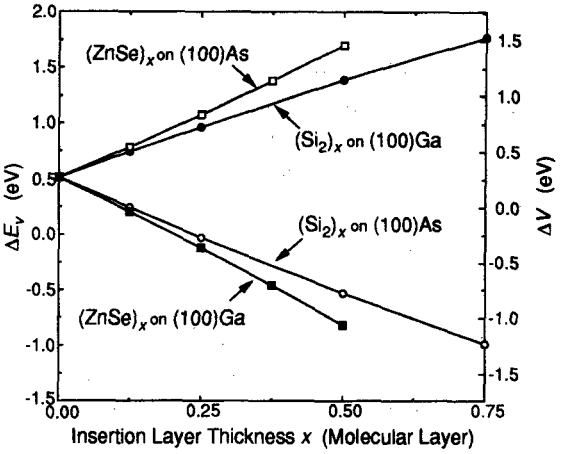

Figure 2: Valence-band discontinuities (ΔE_v) and dipoles (ΔV) at the (100) GaAs/AlAs interfaces with the $(\mathrm{ZnSe})_x$ insertion layer and those with the $(\mathrm{Si}_2)_x$ insertion layer [3]. (100)As and (100)Ga indicate the As-terminated and the Ga-terminated GaAs, respectively.

4. CONCLUSIONS

We have theoretically analyzed the valence-band discontinuity (ΔE_v) at the (100) GaAs/AlAs interfaces with the $(\mathrm{ZnSe})_x$ insertion layers ($0 \leq x \leq 0.5$) by using the self-consistent sp^3s^* tight-binding method. With the $(\mathrm{ZnSe})_{0.5}$ insertion layer (the maximum x in the present study), ΔE_v is calculated to be 1.70 eV (on the As-terminated GaAs) and -0.82 eV (on the Ga-terminated GaAs), which are larger by 1.19

eV and smaller by 1.33 eV, respectively, than $\Delta E_v = 0.51$ eV (no insertion layers). The magnitude of the ΔE_v change due to the $(ZnSe)_x$ insertion layer is slightly larger than that due to the $(Si_2)_x$ insertion layer. The present result predicts a possibility of the artificial control of ΔE_v at the (100) GaAs/AlAs interface by the insertion of the $(ZnSe)_x$ layer.

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