Control of band discontinuities at (100) GaAs/AlAs interfaces by ZnSe insertion layers: Comparison with Si insertion layers

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We have theoretically analyzed the valence-band discontinuity ΔE_v at the (100) GaAs/AlAs interfaces with the $(\mathrm{ZnSe})_x$ insertion layers ($0 \leqslant x \leqslant 0.5$ ML) by using a self-consistent sp^3s^* tight-binding method. The $(\mathrm{ZnSe})_x$ layer inserted on As-terminated GaAs and that inserted on Ga-terminated GaAs are examined. At $x=0.5$, we obtained $\Delta E_v = 1.70$ eV (-0.82 eV) for As- (Ga-) terminated GaAs, while $\Delta E_v = 0.51$ eV at $x=0$. ΔE_v is controlled artificially by the ZnSe-induced dipole. The $(\mathrm{ZnSe})_x$ insertion has an advantage over the $(\mathrm{Si}_2)_x$ insertion, because the change in ΔE_v at high x is larger for the former than for the latter. [S0163-1829(97)05244-2]

The band discontinuities at the (100) GaAs/AlAs interfaces with group-IV-impurity insertion layers (Ge,Si) have been investigated theoretically[1–6] and experimentally[1,7] in order to control the technologically important interfaces. The insertion of the Ge double layer at the interface changes the band discontinuity by the order of 1 eV as shown by the theoretical calculations.[2–5] Due to the Ge insertion, the interface atomic arrangement changes from [-Ga-As-*Ga*-*As*-Al-As-] to [-Ga-As-*Ge*-*Ge*-Al-As-]. According to Harrison's theoretical alchemy model,[8] the Ge double layer at the interface can be regarded as arising from the transfer of protons from the *As* layer to the adjacent *Ga* layer ($Ga \leftarrow As$), and thus inducing the Ge^+-Ge^- dipole, by which the band discontinuity is controlled.[2] Using a similar argument, the insertion of the Si double layer changes the band discontinuity due to the Si^+-Si^- dipole, as calculated theoretically in Refs. 5 and 6. The experiments for the Si insertion were carried out by Sorba *et al.*[7] On the other hand, isoelectronic-impurity insertion layers, such as In (group III) and P (group V), have little effect on the band discontinuity.[9]

Here we propose the "ZnSe double layer" (group II-VI) as another possible impurity layer that can control the band discontinuity. In this case, the interface atomic arrangement is [-Ga-As-*Zn*-*Se*-Al-As-]. Again according to the Harrison model,[8] the ZnSe layer at the interface can be regarded as arising from the proton transfer from the *Ga* layer to the adjacent *As* layer ($Ga \rightarrow As$), and inducing the Zn^--Se^+ dipole. The direction of the proton transfer for the ZnSe double layer is opposite to that for the Ge (and Si) double layer. The band discontinuity is expected to be controlled by the Zn^--Se^+ dipole.

In the microscopic-capacitor (MC) model,[2,5] a double layer inserted at the interface is modeled by a parallel-plate capacitor. This model gives the dipole *induced* by a double layer ΔV^{ind} as $\Delta V^{\mathrm{ind}} = 2\pi e^2 / a \varepsilon_i^{\mathrm{eff}}$ for the (100) interface, where e is the magnitude of the electron charge, a is the GaAs lattice constant, and $\varepsilon_i^{\mathrm{eff}}$ is the effective dielectric constant of the inserted semiconductor.[2,5] We can expect ($\varepsilon_i^{\mathrm{eff}}$ for ZnSe)$<$($\varepsilon_i^{\mathrm{eff}}$ for Si)$<$($\varepsilon_i^{\mathrm{eff}}$ for Ge), considering the differences among the bulk dielectric constants; (5.9 for ZnSe)$<$(12.0 for Si)$<$(16.0 for Ge). Accordingly, the dipole induced by the ZnSe double layer is expected to be larger than that induced by the group-IV (Ge, Si) double layer, because $\Delta V^{\mathrm{ind}} \propto (\varepsilon_i^{\mathrm{eff}})^{-1}$. *The change in the band discontinuity is expected to be larger for the ZnSe insertion than for the group-IV insertion*. However, until now, theoretical and experimental investigations for the ZnSe insertions have not been carried out, in spite of the fact that the growth of ZnSe on GaAs is possible in the present growth technology.[10]

In this study, we theoretically analyze the valence-band discontinuity ΔE_v at the (100) GaAs/AlAs interface with the $(\mathrm{ZnSe})_x$ insertion layers ($0 \leqslant x \leqslant 0.5$ ML) to clarify how large the insertion layers can control ΔE_v. The theoretical calculations of ΔE_v are carried out by using a self-consistent tight-binding (SC-TB) method[3,4,6,9,11] with the sp^3s^* basis.[12] The x dependence of ΔE_v for the $(\mathrm{ZnSe})_x$ insertion obtained in the present study is compared with that for the $(\mathrm{Si}_2)_x$ insertion obtained in our previous study by using the same SC-TB method[6] to clarify whether the change in ΔE_v is larger for the former than for the latter as we expect. We evaluate $\varepsilon_i^{\mathrm{eff}}$ for ZnSe, GaAs, and Si, by fitting the x dependence of ΔE_v in the MC model to that in the SC-TB result, and discuss how the difference in $\varepsilon_i^{\mathrm{eff}}$ affects the x dependence of ΔE_v.

The sp^3s^* tight-binding parameters for GaAs, AlAs, and ZnSe, are taken from the values of Vogl, Hjalmarson, and Dow.[12] The spin-orbit coupling is not included. In the calculations of ΔE_v by using the SC-TB method,[3,4,6,9,11] the atomic-orbital energies are shifted repeatedly according to the changes in the electrostatic potentials induced on the atomic planes, as proposed by Muñoz, Sánchez-Dehesa, and Flores.[11] The $(\mathrm{GaAs})_6/(\mathrm{AlAs})_6$ [100] superlattice is used as a model of the (100) GaAs/AlAs interface. A lattice strain due to the $(\mathrm{ZnSe})_x$ insertion is neglected, because ZnSe is nearly lattice matched to GaAs. Details of the method are described in Ref. 6.

In Ref. 6, we calculated ΔE_v at the (100) GaAs/AlAs interface with no insertion layers (i.e., $x=0$) by using the above method. Figure 1(a) shows the potential profile at the interface for $x=0$ [adapted from Fig. 2(a) in Ref. 6]. 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 average potential in GaAs minus that in AlAs, is 0.27 eV. ΔE_v is obtained as[6]

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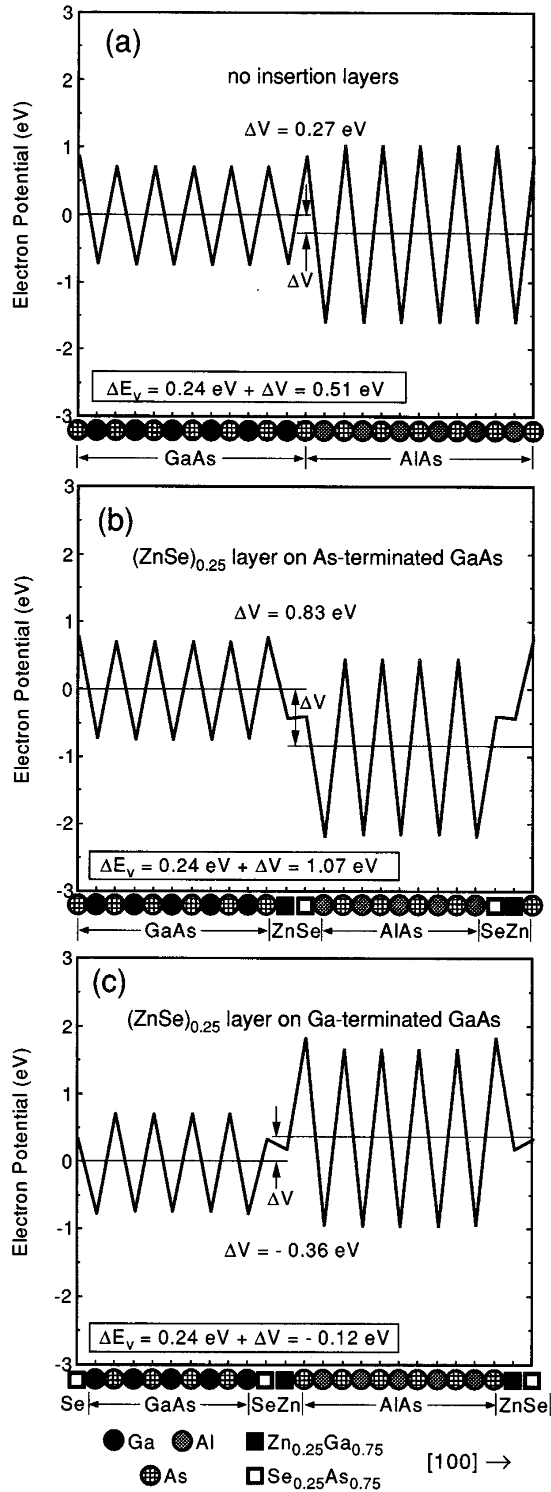

FIG. 1. Potential profiles at the (100) GaAs/AlAs interfaces with (a) no insertion layers, (b) the $(\mathrm{ZnSe})_{0.25}$ layer on As-terminated, and (c) the $(\mathrm{ZnSe})_{0.25}$ layer on Ga-terminated GaAs. ΔV is the dipole.

$$\Delta E_v = \Delta E_v^0 + \Delta V. \tag{1}$$

Here, ΔE_v^0 $(=0.24\,\mathrm{eV})$ is the ''natural'' valence-band discontinuity,[13] which is defined as the valence-band discontinuity when the two semiconductors are separated (i.e., $\Delta V=0$). From Eq. (1), we obtained $\Delta E_v = 0.51$ eV at the interface for $x=0$.[6]

If the $(\mathrm{ZnSe})_x$ insertion layer changes ΔV, it changes ΔE_v according to Eq. (1). By indicating the x-dependence of ΔE_v and ΔV explicitly, Eq. (1) can be rewritten as $\Delta E_v(x) = \Delta E_v^0 + \Delta V(x)$. The dipole *induced* by an insertion layer ΔV^{ind} is defined as $\Delta V^{\mathrm{ind}}(x) \equiv \Delta V(x) - \Delta V(0) = \Delta E_v(x) - \Delta E_v(0)$. This equation can be further rewritten as

$$\Delta E_v(x) = \Delta E_v(0) + \Delta V^{\mathrm{ind}}(x), \tag{2}$$

which shows clearly that the induced dipole can control ΔE_v.

We calculated ΔE_v [or $\Delta E_v(x)$] at the (100) GaAs/AlAs interface with the $(\mathrm{ZnSe})_x$ insertion layers with the thickness $0 \leq x \leq 0.5$ ML, because most of the experiments for the Si insertion concentrated on ΔE_v in this thickness range.[6,7] We assume that the $(\mathrm{ZnSe})_x$ layer is inserted as {-Ga-As-$[Zn_xGa_{1-x}]$-$[Se_xAs_{1-x}]$-Al-As-} and {-As-Ga-$[Se_xAs_{1-x}]$-$[Zn_xGa_{1-x}]$-As-Al-}, on As-terminated and Ga-terminated GaAs, respectively.[14] The $[Zn_xGa_{1-x}]$-$[Se_xAs_{1-x}]$ double layer (on As-terminated GaAs) and its inverted $[Se_xAs_{1-x}]$-$[Zn_xGa_{1-x}]$ double layer (on Ga-terminated GaAs) are the *alloy layers* which consist of the $(\mathrm{ZnSe})_x$ *insertion layer* and the $(\mathrm{GaAs})_{1-x}$ *host layer*. The $(\mathrm{ZnSe})_x$ layer arises from the proton transfer from the *Ga* layer to the adjacent *As* layer with a fraction x, and induces the $(Zn^-\text{-}Se^+)_x$ dipole (As-terminated) and the $(Se^+\text{-}Zn^-)_x$ dipole (Ga-terminated), according to Harrison's model.[8] Since the polarity of the dipole on As-terminated GaAs is opposite that on Ga-terminated GaAs, the opposite effect on 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 As-terminated and 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 (Ref. 6) at the interface for $x=0$. The insertion of the $(\mathrm{ZnSe})_x$ layer changes ΔE_v significantly even for $x=0.25$ ML.

Figure 2 shows ΔE_v (and ΔV) at the (100) GaAs/AlAs interfaces with the $(\mathrm{ZnSe})_x$ insertion layer. As shown in the figure, ΔE_v increases (decreases) according to a linear relation with x for As- (Ga-) terminated GaAs at very low x. The dashed straight line indicates the linear relation. However, ΔE_v changes *more* than the linear relation at high x, deviating from the above straight line with a positive (negative) curvature. For $x=0.5$, we obtained $\Delta E_v = 1.70$ eV (-0.82 eV) for As- (Ga-) terminated GaAs, which is larger by 1.19 eV (smaller by 1.33 eV) than $\Delta E_v = 0.51$ eV for $x=0$. 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. The sign of the change in ΔE_v depends on a terminated plane of GaAs, and the magnitude of the change depends on x, clearly showing that the ZnSe-induced dipole controls ΔE_v.

Figure 2 also shows 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. 6.) Due to the $(\mathrm{Si}_2)_x$ insertion, ΔE_v decreases (increases) according to a linear relation with x for As- (Ga-) terminated GaAs at very low x, like the $(\mathrm{ZnSe})_x$ insertion. However, unlike the $(\mathrm{ZnSe})_x$ in-

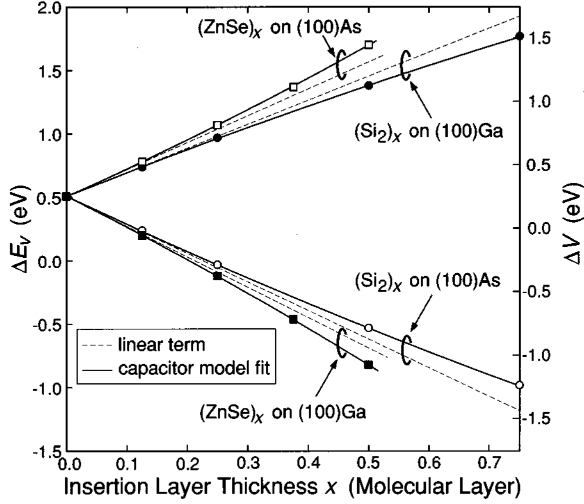

FIG. 2. Valence-band discontinuities ΔE_v (and dipoles ΔV) at the (100) GaAs/AlAs interfaces as a function of the insertion layer thickness x. The open and full squares indicate ΔE_v for the $(ZnSe)_x$ insertion layer on As- and Ga-terminated GaAs, respectively, calculated by using the SC-TB method in the present study. The open and full circles indicate ΔE_v for the $(Si_2)_x$ insertion layer on As- and Ga-terminated GaAs, respectively, calculated by using the SC-TB method in Ref. 6. The solid curves indicate ΔE_v calculated by using the MC model[5] with the *adjusted* effective dielectric constants ε^{eff}. The dashed straight lines indicate the linear terms of ΔE_v in the MC model.

sertion, ΔE_v changes *less* than the linear relation at high x. Consequently, at high x, the change in ΔE_v with the $(ZnSe)_x$ insertion is significantly larger than that with the $(Si_2)_x$ insertion (by ≈ 0.3 eV for $x=0.5$ ML) owing to the different x dependence of ΔE_v. The $(ZnSe)_x$ insertion has an advantage over the $(Si_2)_x$ insertion in that it causes a larger change in ΔE_v.

In Fig. 2, the larger change in ΔE_v with the $(ZnSe)_x$ insertion is partly due to the larger slope of the linear relation compared to the slope with the $(Si_2)_x$ insertion. However, in the MC model (described below), the slope is defined by the effective dielectric constant of GaAs independent of insertion layers. The small difference in the slope between the two insertion layers in Fig. 2 is mainly related to the accuracy of the SC-TB calculation, but it does not affect the tendency of the ΔE_v change.

In the MC model,[2,5] a double layer inserted at the interface is modeled by a parallel-plate capacitor: the $(Zn^{-}\text{-}Se^{+})_x$ capacitor and $(Si^{+}\text{-}Si^{-})_x$ capacitor in the present study. The distance between the two plates is one (100) interplanar spacing $a/4$, and the charge on the plates (before dielectric screening) depends linearly on x. From simple electrostatics, the magnitude of the dipole induced by a double layer $\Delta V^{\text{ind}}(x)$, used in Eq. (2), is expressed by Peressi *et al.*[5] as $|\Delta V^{\text{ind}}(x)| = 2\pi e^2 x / a\varepsilon_a^{\text{eff}}(x)$. Here $\varepsilon_a^{\text{eff}}(x)$ is the *effective* dielectric constant of the *alloy layer* at the interface which consists of the *insertion layer* $[(ZnSe)_x$ or $(Si_2)_x]$ and *host layer* $[(GaAs)_{1-x}]$. $\varepsilon_a^{\text{eff}}(x)$ is given as[5] $\varepsilon_a^{\text{eff}}(x)^{-1} = (1-x)(\varepsilon_h^{\text{eff}})^{-1} + x(\varepsilon_i^{\text{eff}})^{-1}$, where $\varepsilon_h^{\text{eff}}$ $(\varepsilon_i^{\text{eff}})$ is the effective dielectric constant of the host (insertion) layer. Using the above equation, $|\Delta V^{\text{ind}}(x)|$ is rewritten as [Eq. (1) in Ref. 5]

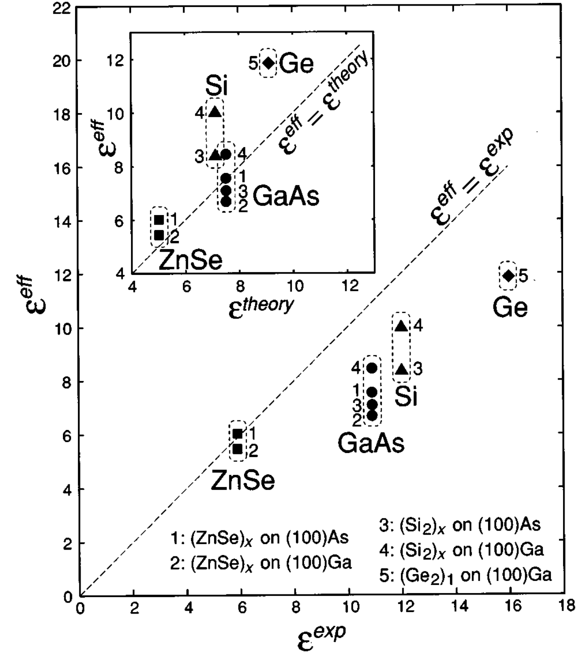

FIG. 3. Effective dielectric constant of insertion layers ε^{eff} vs. experimental dielectric constant of bulk semiconductors ε^{exp}, for ZnSe, GaAs, Si, and Ge. For labels 1–4, ε^{eff} is obtained by fitting ΔE_v of the MC model[5] to that of the SC-TB method, as shown in Fig. 2. For label 5, ε^{eff} is obtained from ΔE_v calculated in Ref. 4. The values of ε^{exp} are taken from Table 4-1 in Ref. 15. The inset shows ε^{eff} vs theoretical dielectric constant of bulk semiconductors $\varepsilon^{\text{theory}}$. The values of $\varepsilon^{\text{theory}}$ are taken from the present study for ZnSe (see the text), and from Ref. 16 for the rest.

$$|\Delta V^{\text{ind}}(x)| = \frac{2\pi e^2 x}{a\varepsilon_h^{\text{eff}}} + \frac{2\pi e^2 x^2}{a}\left(\frac{1}{\varepsilon_i^{\text{eff}}} - \frac{1}{\varepsilon_h^{\text{eff}}}\right). \tag{3}$$

It is indicated from Eqs. (2) and (3) that ΔE_v changes with x according to the linear term $2\pi e^2 x/a\varepsilon_h^{\text{eff}}$ of Eq. (3) at very low x, and changes *more* (*less*) than the linear term at high x if $\varepsilon_i^{\text{eff}} < \varepsilon_h^{\text{eff}}$ $(\varepsilon_i^{\text{eff}} > \varepsilon_h^{\text{eff}})$. The relative magnitude of $\varepsilon_i^{\text{eff}}$ and $\varepsilon_h^{\text{eff}}$ determines how ΔE_v deviates from the linearity. It should be noted that $\varepsilon_i^{\text{eff}}$ and $\varepsilon_h^{\text{eff}}$ (in general ε^{eff}) may not be exactly equal to the corresponding *bulk* dielectric constants, because the capacitor is too thin $(a/4)$ to be regarded as bulk. Next, we quantitatively deduce the values of ε^{eff} by fitting the ΔE_v curve calculated by the MC model to the ΔE_v values calculated by the SC-TB method by adjusting ε^{eff}.

In Fig. 2, the solid curves indicate ΔE_v calculated by the MC model [Eqs. (2) and (3)], which are fitted, by adjusting ε^{eff}, to the ΔE_v values at $x=0.25$ and 0.50 ML calculated by the SC-TB method, for the $(ZnSe)_x$ and $(Si_2)_x$ insertions on As- and Ga- terminated GaAs. (A set of $\varepsilon_i^{\text{eff}}$ and $\varepsilon_h^{\text{eff}}$ is obtained by fitting procedure for one ΔE_v curve.) The obtained values of ε^{eff} $[\varepsilon_i^{\text{eff}}(\text{ZnSe}), \varepsilon_i^{\text{eff}}(\text{Si}), \varepsilon_h^{\text{eff}}(\text{GaAs})]$ are plotted in Fig. 3. The dashed straight lines in Fig. 2 indicate ΔE_v calculated by the linear term of Eq. (3) in the MC model.

Figure 3 shows ε^{eff} versus experimental dielectric constant of bulk semiconductors ε^{exp}, for ZnSe, GaAs, Si, and Ge. For Ge, ε^{eff} is obtained from ΔE_v at the interface with

the $(Ge_2)_1$ insertion layer on Ga-terminated GaAs [$\Delta E_v = 1.86$ eV, and $\Delta V^{ind}(1.0) = 2\pi e^2/a\varepsilon_i^{eff} = 1.35$ eV, here $\varepsilon_i^{eff} = \varepsilon^{eff}(Ge)$], which was calculated by using the SC-TB method in Ref. 4.

First let us discuss the difference between ε^{eff} and ε^{exp} for each semiconductor. As shown in Fig. 3, for each semiconductor except ZnSe, ε^{eff} is smaller than ε^{exp} by a factor 0.6~0.8, while the relative magnitude of ε^{exp} (ZnSe<GaAs<Si<Ge) is clearly reproduced in that of ε^{eff}. The one reason for the difference, $\varepsilon^{eff} < \varepsilon^{exp}$, can be related to the fact that the sp^3s^* tight-binding theories[13,16,17] usually underestimate the dielectric constant even for bulk semiconductors. For example, the theoretical dielectric constant of bulk ε^{theory} is calculated as $\varepsilon^{theory} = 7.5$ (GaAs), 7.1 (Si), 9.1 (Ge) by Durán *et al.*,[16] $\varepsilon^{theory} = 7.2$ (Si) by Graf and Vogl,[17] and $\varepsilon^{theory} = 5.03$ (ZnSe), 7.65 (GaAs) by us in the present study,[18] which are smaller than the corresponding ε^{exp} by a factor 0.6~0.85. The above values of ε^{theory} were obtained as a long-wavelength limit of dielectric function by using the sp^3s^* basis. Some corrections to Vogl's sp^3s^* parametrization, like orbital nonorthogonality, may increase the values of ε^{theory}.[13] The inset of Fig. 3 shows ε^{eff} versus ε^{theory}, where ε^{eff} shows a better numerical correlation with ε^{theory} than with ε^{exp}. It should be noted that the comparison between the ZnSe-induced dipole and the Si-induced dipole is valid as long as we use the same sp^3s^* parametrization for both, although the underestimation of ε^{eff} (i.e., underestimation of screening) leads to the overestimation of $|\Delta V^{ind}|$. Thus the present calculation mainly gives the tendency for the dipole change.[19]

In Fig. 3, we can also see that ε^{eff} for each semiconductor does not take a single value, but takes slightly different values depending on the interface structures such as a terminated plane of GaAs. This fact clearly indicates that ε^{eff} is not exactly a bulk quantity, which can be another reason f
rthe difference between ε^{eff} and ε^{exp}.

Next let us discuss the difference in ε^{eff} between the semiconductors and the effect on the x dependence of ΔE_v. For the $(ZnSe)_x$ insertions, ε^{eff} of ZnSe is calculated to be 20.0% (18.3%) smaller than ε^{eff} of GaAs for As- (Ga-) terminated GaAs (on average, 19.2% smaller), as shown in Fig. 3. In other words, ε^{eff} of the insertion layer is smaller than that of the host; i.e., $\varepsilon_i^{eff} < \varepsilon_h^{eff}$. This is the source of the result in Fig. 2 that ΔE_v changes *more* than the linear relation at high x for the $(ZnSe)_x$ insertion, as already indicated by Eqs. (2) and (3). On the other hand, for the $(Si_2)_x$ insertion, ε^{eff} of Si is calculated to be 18.2% (18.4%) larger than ε^{eff} of GaAs for As- (Ga-) terminated GaAs (on average, 18.3% larger); i.e., $\varepsilon_i^{eff} > \varepsilon_h^{eff}$. This is the source of the result that ΔE_v changes *less* than the linear relation at high x, again by Eqs. (2) and (3). Such x dependence for the $(Si_2)_x$ insertion was already shown by Peressi *et al.*[5] From the above analysis, we conclude that the larger change in ΔE_v at high x for the $(ZnSe)_x$ insertion over the $(Si_2)_x$ insertion is the consequence of smaller ε^{eff} of ZnSe: (ε^{eff} of ZnSe) < (ε^{eff} of GaAs) < (ε^{eff} of Si).

In conclusion, we have theoretically analyzed ΔE_v at the (100) GaAs/AlAs interfaces with the $(ZnSe)_x$ insertion layers ($0 \leq x \leq 0.5$ ML) by using the sp^3s^* SC-TB method. ΔE_v increases (decreases) according to a linear relation with x for As- (Ga-) terminated GaAs at very low x, and changes *more* than the linear relation at high x. At $x = 0.5$, we obtained $\Delta E_v = 1.70$ eV (-0.82 eV) for As- (Ga-) terminated GaAs, while $\Delta E_v = 0.51$ eV at $x = 0$. ΔE_v is controlled artificially by the ZnSe-induced dipole. ε^{eff} of the inserted ZnSe is 19.2% smaller than ε^{eff} of GaAs causing the excess change in ΔE_v over the linearity at high x. The $(ZnSe)_x$ insertion has an advantage over the $(Si_2)_x$ insertion, because the change in ΔE_v at high x is larger for the former than for the latter.

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[18] We calculated ε^{theory} using the method described in Sec. III of Ref. 16, where ε^{theory} is obtained from the dielectric behavior of a semiconductor *homo*-interface when an initial perturbation, Eq. (6) of Ref. 16, is applied at the interface. We used $(ZnSe)_6/(ZnSe)_6$ and $(GaAs)_6/(GaAs)_6$ [100] superlattices for the calculation.
[19] In the present study, ε^{theory} of AlAs does not relate to the dipole ΔV^{ind} explicitly because the interface *alloy layer* does not include AlAs, but this value, together with ε^{theory} of GaAs, defines $\Delta E_v(0)$ (Ref. 16).