PHYSICAL REVIEW B VOLUME 46, NUMBER 4 15 JULY 1992-II

Donor impurity states on structured semiconductor interfaces

Hong Sun* and Shi-Wei Gu
Chinese Center of Advanced Science and Technology (World Laboratory), Beijing 100080, The People's Republic of China and International Center for Material Physics, Academia Sinica, Shenyang 110015, The People's Republic of China

(Received 7 November 1991)

Ground-state energies of shallow states of donor impurities on periodically structured interfaces formed by two semiconductors, such as $GaAs/Ga_{1-x}Al_xAs$ and Si/SiO_2 interfaces, are calculated variationally with the approximation that interfaces represent infinitely high potential barriers. The results show that the ground-state energies of the interface impurity states can be strongly affected by interface structures in $GaAs/Ga_{1-x}Al_xAs$ lateral surface superlattices produced by molecular-beam-epitaxy growth of AlAs/GaAs fractional-layer superlattices on [001] vicinal GaAs substrates and on SiO_2/Si interfaces for Si with (001) orientation. The effects of the interface defects on the interface impurity states are negligible for Si/SiO_2 interfaces when the density of interface defects is less than $10^{10}/cm^2$.

I. INTRODUCTION

Shallow states of donor impurities on semiconductor interfaces have long been the focus of extensive studies by many authors, for a number of properties of semiconductor-interface devices are strongly influenced by these interface impurity states.[1-8] And in recent years, impurity states in $GaAs/Ga_{1-x}Al_xAs$ quantum wells with impurity ions on or near the $GaAs/Ga_{1-x}Al_xAs$ interface have also been extensively studied.[9-14]

Most of these studies assumed that semiconductor interfaces are ideally planar. In realistic devices, however, it is almost impossible to fabricate ideally planar semiconductor interfaces due to environmental fluctuations and mechanical control inaccuracy in the process of device manufacturing. Deviations of semiconductor interfaces from planar ones will modify results predicating the energy levels of interface impurity states calculated with semiconductor interfaces that are assumed to be planar. Recently, the idea of lateral surface superlattices[15-22] (LSSL's) has been put forward where periodic structures are built artificially on interfaces of two-dimensional electronic systems, such as $GaAs/Ga_{1-x}Al_xAs$ quantum wells and Si/SiO_2 MOS structures. With the method of molecular-beam-epitaxy (MBE) growth of AlAs/GaAs fractional-layer superlattices on [001] vicinal GaAs substrates, LSSL's with lateral periods as short as 100 Å can be obtained, which are about the same order of magnitude as the Bohr radius of interface impurity states on $GaAs/Ga_{1-x}Al_xAs$ interfaces. Detectable changes on the energy levels of interface impurity states are expected due to periodically structured interfaces.

In this paper, we report the calculation of shallow states of donor impurities on periodically structured semiconductor interfaces which deviate slightly from planes. We intend to study in what way and to what extent periodically structured interfaces will change the energy levels of interface impurity states. In the next section, we present the theory we used to calculate the ground-state energies of interface impurity states. The numerical results and discussion are given in the final section.

II. THEORY

For simplicity, we consider an interface formed by two semiconductors, such as $GaAs/Ga_{1-x}Al_xAs$, GaAs/vacuum, Si/SiO_2, and Si/vacuum interfaces, with a donor impurity ion located on the interface. The structured interface is assumed to be cosine shaped, given by

$$z=f(x,y)=h\cos\frac{x}{a}\cos\frac{y}{b}\ . \tag{1}$$

Since by Fourier transformation, any structured interface can be considered to be the superposition of interfaces given by Eq. (1) with different a and b, the results of our calculation will give indications on the effects of structured interfaces on interface impurity states for general interface shapes. For small interface structures, we must have $h \ll \bar{z}$, where $\bar{z}$ is the expectation value of the electron distance from the interface. Furthermore, we assume that the semiconductor interface represents an infinitely high potential barrier, which confines the electron within semiconductor I, say within GaAs for $GaAs/Ga_{1-x}Al_xAs$ or GaAs/vacuum interfaces and within Si for Si/SiO_2 or Si/vacuum interfaces. This approximation is well satisfied for GaAs/vacuum, Si/SiO_2, and Si/vacuum interfaces and for $GaAs/Ga_{1-x}Al_xAs$ interface with $x>0.2$. The Hamiltonian for the interface impurity state reads

$$H=-\frac{\hbar^2}{2}\left[\frac{1}{m_x}\frac{\partial^2}{\partial x^2}+\frac{1}{m_y}\frac{\partial^2}{\partial x^2}+\frac{1}{m_z}\frac{\partial^2}{\partial x^2}\right]+V(\mathbf{r}) \quad \text{for } z>f(x,y)\ , \tag{2}$$

where for GaAs $m_x=m_y=m_z$ and for Si with [001] orientation $m_x=m_y=m_t$ and $m_z=m_l$. The electron wave function $\psi(\mathbf{r})$ satisfies the boundary condition

 ©1992 The American Physical Society

$$\psi(\mathbf{r})|_{z=f(x,y)^+}=0\ , \tag{3}$$

where we have assumed that the electron is confined within semiconductor I, which occupies space $z>f(x,y)$ with $z=f(x,y)$ defining the structured interface [see Eq. (1)]. The potential $V(\mathbf{r})$ acting upon the electron consists of (i) the direct Coulombic interaction between the electron and donor impurity ion, (ii) the image potential induced by the ion, and (iii) the image potential induced by the electron itself. $V(\mathbf{r})$ can be obtained by solving the static Poisson equation.[23] Up to the first order in the interface deviation from the planar interfaces, $V(\mathbf{r})$, is given by[23]

$$V(\mathbf{r})=-\frac{e^2}{\bar{\epsilon}|\mathbf{r}-\mathbf{r}_i|}+Q\frac{e^2}{4\epsilon_1 z}+Q\frac{e^2}{2\pi\epsilon_1}\int d\boldsymbol{\rho}' f(x',y')\frac{R_1(\boldsymbol{\rho}'-\boldsymbol{\rho})^2+R_2z^2}{[(\boldsymbol{\rho}'-\boldsymbol{\rho})^2+z^2]^3}$$
$$-Q\frac{e^2}{\pi\epsilon_1}\int d\boldsymbol{\rho}' f(x',y')\frac{R_1(\boldsymbol{\rho}'-\boldsymbol{\rho})\cdot(\boldsymbol{\rho}'-\boldsymbol{\rho}_i)+R_2zz_i}{[(\boldsymbol{\rho}'-\boldsymbol{\rho})^2+z^2]^{3/2}[(\boldsymbol{\rho}'-\boldsymbol{\rho}_i)^2+z_i^2]^{3/2}}\ , \tag{4}$$

where ϵ_1 (ϵ_2) is the dielectric constant of semiconductor I (II), $\mathbf{r}_i=(\boldsymbol{\rho}_i,z_i)$ is the position vector of the donor impurity on the interface, and

$$\boldsymbol{\rho}=(x,y),\quad \bar{\epsilon}=\frac{\epsilon_1+\epsilon_2}{2}\ ,$$
$$R_1=\frac{\epsilon_1}{\epsilon_1+\epsilon_2}\ ,\quad R_2=\frac{\epsilon_2}{\epsilon_1+\epsilon_2}\ ,\quad Q=\frac{\epsilon_1-\epsilon_2}{\epsilon_1+\epsilon_2}\ . \tag{5}$$

From the variation method,[24] the ground-state energy of the impurity state is given by the minimum of the following quantity:

$$F=\int_{-\infty}^{\infty}dx\,dy\int_{f(x,y>}^{\infty}dz\,\psi^*(H\psi)\times\left[\int_{-\infty}^{\infty}dx\,dy\int_{f(x,y>}^{\infty}dz\,\psi^*\psi\right]^{-1}\ , \tag{6}$$

where the trial wave function ψ satisfies the boundary condition (3). Now we introduce the following coordinate transformation which transforms space $\mathbf{r}$ to space $\tilde{\mathbf{r}}$:

$$\tilde{x}=x-x_i\ ,$$
$$\tilde{y}=y-y_i\ , \tag{7}$$
$$\tilde{z}=\left[z-h\cos\frac{x}{a}\cos\frac{y}{b}\right]\Big/\gamma$$

with $\gamma=\sqrt{m_t/m_l}$. In space $\tilde{\mathbf{r}}$, the structured interface $z=f(x,y)$ is transformed to a planar interface at $\tilde{z}=0$. The quantity F becomes

$$F=\int_{-\infty}^{\infty}d\tilde{x}\,d\tilde{y}\times\int_0^{\infty}d\tilde{z}|J(\tilde{x},\tilde{y},\tilde{z})|\tilde{\psi}^*(H_{\text{eff}}\tilde{\psi})\times\left[\int_{-\infty}^{\infty}d\tilde{x}\,d\tilde{y}\int_0^{\infty}d\tilde{z}|J(\tilde{x},\tilde{y},\tilde{z})|\tilde{\psi}^*\tilde{\psi}\right]^{-1}$$
$$=\int_{-\infty}^{\infty}d\tilde{x}\,d\tilde{y}\int_0^{\infty}d\tilde{z}\,\tilde{\psi}^*(H_{\text{eff}}\tilde{\psi})\ , \tag{8}$$

where $J(\tilde{x},\tilde{y},\tilde{z})$ is the Jacobian determinant[25] introduced into the integration when transforming from coordinate system (x,y,z) to $(\tilde{x},\tilde{y},\tilde{z})$. To obtain the last result in Eq. (8), we notice that for the coordinate transformation (7), $J(\tilde{x},\tilde{y},\tilde{z})=\gamma^{-1}$, and we have also required that $\tilde{\psi}$ be normalized in space $\tilde{\mathbf{r}}$. In what follows, we remove the tilde on $\tilde{\psi}$ and $\tilde{\mathbf{r}}$ to simplify the notation. But one must keep in mind that we are working in the transformed space

$$H_{\text{eff}}=H_0+H_1\ , \tag{9}$$

where

$$H_0=-\frac{\hbar^2}{2m_e}\nabla_{\mathbf{r}}^2-\frac{e^2}{\bar{\epsilon}\sqrt{\rho^2+\gamma^2z^2}}+Q\frac{e^2}{4\epsilon_1\gamma z} \tag{10}$$

and

$$H_1=\frac{\hbar^2}{2m_e}\left[\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right]f(x+x_i,y+y_i)\frac{\partial}{\gamma\partial z}-2\frac{\partial}{\partial x}f(x+x_i,y+y_i)\frac{\partial^2}{\gamma\partial x\partial z}\right.$$
$$\left.-2\frac{\partial}{\partial y}f(x+x_i,y+y_i)\frac{\partial^2}{\gamma\partial y\partial z}\right]-f(x+x_i,y+y_i)Q\frac{e^2}{4\epsilon_1\gamma^2z^2}$$
$$+2\frac{\gamma e^2z}{\epsilon_1(\rho^2+\gamma^2z^2)^{3/2}}[R_1f(x+x_i,y+y_i)-R_2f(x_i,y_i)]+Q\frac{e^2}{2\pi\epsilon_1}\int d\boldsymbol{\rho}' f(x',y')\frac{R_1(\boldsymbol{\rho}'-\boldsymbol{\rho}-\boldsymbol{\rho}_i)^2+R_2\gamma^2z^2}{[(\boldsymbol{\rho}'-\boldsymbol{\rho}-\boldsymbol{\rho}_i)^2+\gamma^2z^2]^3}$$
$$-Q\frac{e^2}{\pi\epsilon_1}\int d\boldsymbol{\rho}' f(x',y')\frac{R_1\boldsymbol{\rho}'\cdot(\boldsymbol{\rho}'-\boldsymbol{\rho}-\boldsymbol{\rho}_i)+R_2\gamma zz_i}{[(\boldsymbol{\rho}'-\boldsymbol{\rho}-\boldsymbol{\rho}_i)^2+\gamma^2z^2]^{3/2}(\rho'^2+z_i^2)^{3/2}} \tag{11}$$

with $m_e = m_x$ for GaAs and $m_e = m_t$ for Si. H_1 is a small perturbation, which is Hermitian and tends to zero as $f(x,y) \to 0$. After the coordinate transformation (7), the boundary condition [Eq. (3)] becomes

$$\psi|_{z=0} = 0 \ . \quad (12)$$

Since H_{eff} is Hermitian, it is easy to prove[24] that F (8) reaches its minimum, which is the ground-state energy of the interface impurity state, when ψ is the ground-state eigenfunction of H_{eff} subject to the boundary condition (12).

The ground-state energy of the effective Hamiltonian H_{eff} (9) is obtained by a variational calculation. First we rewrite H_0 (10) as

$$H_0 = -\frac{\hbar^2}{2m_e}\nabla_{\mathbf{r}}^2 - \frac{\alpha e^2}{\bar{\epsilon} r} + Q\frac{e^2}{4\epsilon_1 \gamma z} + \Delta V(\mathbf{r}) \quad (13)$$

with

$$\Delta V(\mathbf{r}) = \frac{\alpha e^2}{\bar{\epsilon} r} - \frac{e^2}{\bar{\epsilon}\sqrt{\rho^2 + \gamma^2 z^2}} \ . \quad (14)$$

The trial wave function is taken as the ground-state wave function of H_0 with $\Delta V(\mathbf{r})$ set equal to zero, that is

$$\psi_g(\mathbf{r},\beta) = \sqrt{2/\pi}\left[\frac{\beta}{a_0}\right]^{5/2} z \exp\left[-\frac{\beta}{a_0}\sqrt{\rho^2 + z^2}\right] , \quad (15)$$

where $a_0 = \hbar^2\bar{\epsilon}/m_e e^2$ is the Bohr radius of the interface impurity state and β is the variational parameter. $\psi_g(\mathbf{r},\beta)$ is normalized in the transformed space and satisfies the boundary condition of (12). The parameter α in H_0 (13) is determined by requiring

$$\langle \psi_g(\mathbf{r},\beta) | \Delta V(\mathbf{r}) | \psi_g(\mathbf{r},\beta) \rangle = 0 \ . \quad (16)$$

The ground-state energy of the interface impurity state we considered is given by

$$E_g = \min_{\beta} \langle \psi_g(\mathbf{r},\beta) | H_{\text{eff}}(\mathbf{r}) | \psi_g(\mathbf{r},\beta) \rangle \ . \quad (17)$$

The trial wave function (15) is expected to be a good one, as long as the energy shifts caused by the structured interfaces are much less than the level spacings between the ground and first-excited interface impurity states.

III. NUMERICAL RESULTS AND DISCUSSIONS

The numerical results for the ground-state energies of interface impurity states are carried out for the following two cases. In case (i), we take $a = b$ in Eq. (1), which represents structurally defective interfaces with a defect density equal to $N = (2\pi a)^{-2}$. And in case (ii), we take $b \to \infty$, which represents one-dimensional periodically structured interfaces, such as those produced by the molecular-beam-epitaxy growth of AlAs/GaAs fractional-layer superlattices on [001] vicinal GaAs substrates. The quantity we calculated is $\delta\tilde{E}_g = (E_g - E_g^{(0)})/|E_g^{(0)}|(z_i/\bar{z})$ as a function of $k = \sqrt{1/a^2 + 1/b^2}$, where E_g and $E_g^{(0)}$ are the ground-state energies of the interface impurity states on the structured interfaces given by Eq. (1) and on planar interfaces, respectively, and $z_i = h\cos(x_i/a)\cos(y_i/b)$ is the position of the impurity ion on the structured interfaces. For case (i), $k = \sqrt{2}/a$, and for case (ii), $k = 1/a$. The numerical results of $\delta\tilde{E}_g(k)$ are found to be nearly the same for the two cases we considered. The numerical results of $\delta\tilde{E}_g$ as functions of a/a_0 are given in Fig. 1 for the case (i) ($a = b$) for (a) GaAs/vacuum, (b) $GaAs/Ga_{1-x}Al_xAs$, (c) Si/vacuum, and (d) Si/SiO_2 interfaces, respectively. The experimental parameters used in the calculation are listed in Table I together with other quantities calculated from them. The results in Fig. 1 also apply for case (ii) ($b \to \infty$), if the unit of the abscissa in Fig. 1 is changed from a/a_0 to $\sqrt{2}a/a_0$.

From Fig. 1, the following points are worth mentioning. The effects of the interface structures on the interface impurity states decrease rapidly with increasing periods of the interface structures. When $a/a_0 > 4$, the effects of the interface structures are negligible for the interfaces we considered. Physically, this is obvious. The periods of interface structures are $d = 2\pi a$, while electrons in the interface impurity states distribute mainly in

TABLE I. The experimental parameters used in the calculation, where ϵ_1 and ϵ_2 are the dielectric constants of semiconductors I and II forming the interface (semiconductor I)/(semiconductor II) [the dielectric constant of $Ga_{1-x}Al_xAs$ is taken with composition $x > 0.3$[11] to ensure the validity of the infinitely high potential barrier approximation (see the test)], and m_t and m_l are the electron band masses of semiconductor I in the directions parallel and normal to the interface. $E_g^{(0)}$ (in meV) is the ground-state energy, $a_0 = \hbar^2\bar{\epsilon}/m_e e^2$ (in Å) is the Bohr radius, and $\bar{z}$ (in Å) is the expectation value of the electron distance from the interface in an interface impurity state on a planar interface, respectively. The experimental parameters are taken from Ref. 26.

Interfaces	ϵ_1	ϵ_2	m_t	m_l	$E_g^{(0)}$	a_0	$\bar{z}$
GaAs/vacuum	12.35	1.0	0.066	0.066	−3.452	53.52	242.5
$GaAs/Ga_{1-x}Al_xAs$	12.35	10.29	0.066	0.066	−1.644	90.77	351.4
Si/vacuum	11.8	1.0	0.190	0.916	−18.93	12.11	27.80
Si/SiO_2	11.8	3.80	0.190	0.916	−15.12	14.76	31.10
Model Si interface	11.8	9.83	0.190	0.916	−10.88	20.47	36.66

a half-sphere with a radius $\bar{r}=\langle \psi_g(\mathbf{r})|r|\psi_g(\mathbf{r})\rangle \cong 5a_0$ centered on impurity ions. When $a/a_0>4$, we have $d/\bar{r}>5$. To an electron in the interface impurity state, the interface is locally planar. The effects of the interface structures on the interface impurity states become important when the periods of the interface structures are reduced to $d/\bar{r}\cong a/a_0<2$. In this region, $\delta\tilde{E}_g$ is negative. When $z_i>0$, that is, with the impurity ions located on parts of the interfaces embedded in semiconductors I, the ground-state energies of the interface impurity states are shifted to a lower level than those with impurity ions located on parts of the interfaces protruding from semiconductors I.

If the impurities are distributed homogeneously on the interfaces, the energy levels of the interface impurity states are broadened into impurity energy bands. If the interactions among impurities can be neglected, the widths E_b of impurity energy bands are given by $E_b/|E_g^{(0)}|=2h|\delta\tilde{E}_g|/\bar{z}$. For Si/SiO_2 interfaces with a height of interface defects $h=5$ Å, we have, from Fig. 1 (d), $E_b/|E_g^{(0)}|=0.5\%$ for a density of interface defects of $N=(2\pi a)^{-2}=10^{10}/cm^2$, $E_b/E_g^{(0)}|=5\%$ for $N=10^{11}/cm^2$, and $E_b/|E_g^{(0)}|=15\%$ for $N=10^{12}/cm^2$. The actual broadenings of the impurity energy bands caused by interface defects in Si/SiO_2 interfaces are expected to be larger than our estimates, because in our calculation we considered only cosine-shaped interface defects which are rather flat defects. Actual Si/SiO_2 interfaces are expected to have sharply structured interface defects, which cause large broadenings of the impurity energy bands. But we believe when the density of interface defects of a Si/SiO_2 interface is less than $10^{10}/cm^2$, the broadenings of the im-

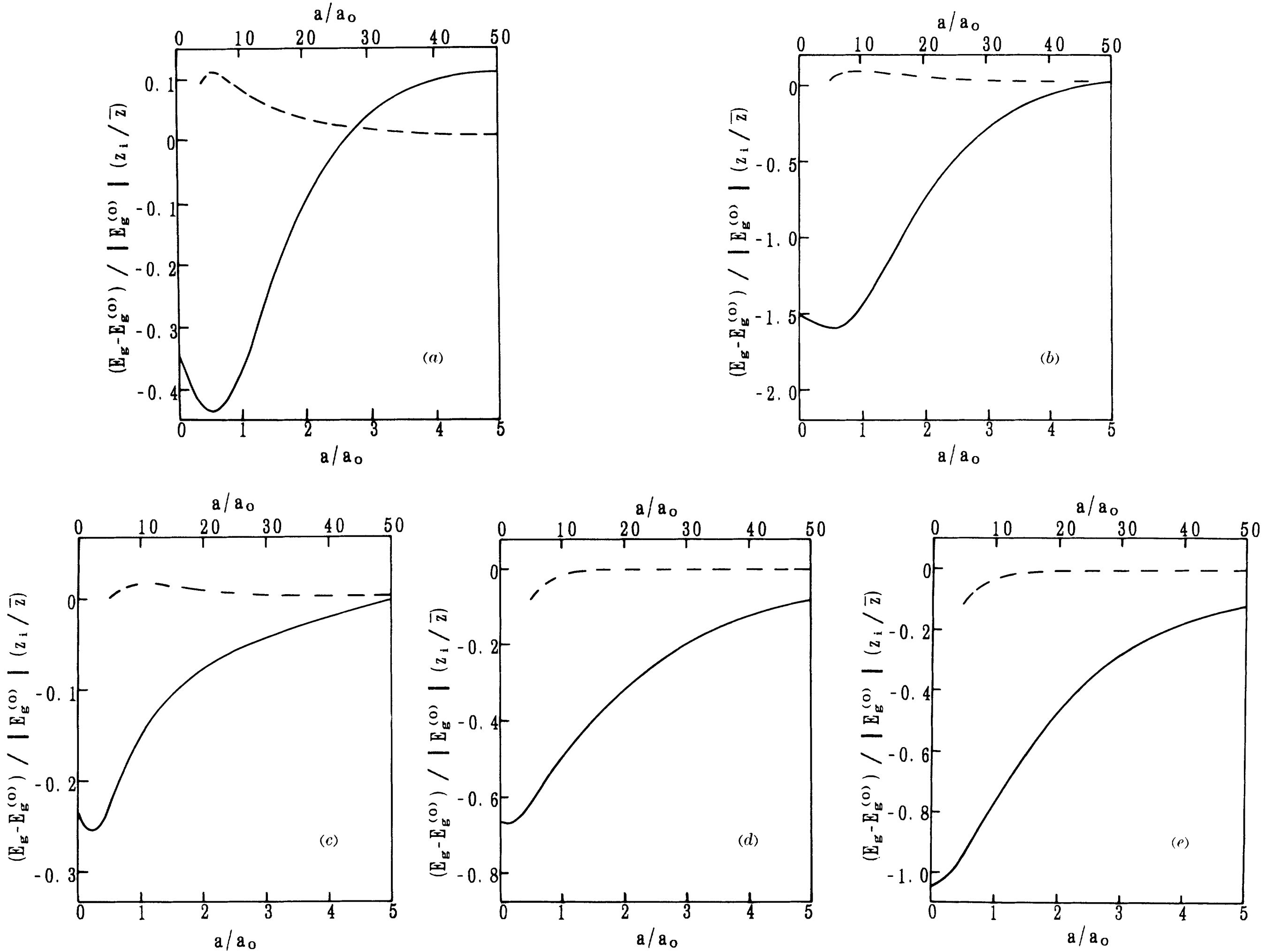

FIG. 1. Shifts $\delta\tilde{E}_g=(E_g-E_g^{(0)})/|E_g^{(0)}|(z_i/\bar{z})$ of the ground-state energies E_g of interface impurity states relative to the ground-state energies $E_g^{(0)}$ of impurity states on planar interfaces, calculated as functions of a/a_0 for periodically structured interfaces defined by $z=h\cos(x/a)\cos(y/b)$, where z_i is the position of the impurity ion on the structured interfaces, $\bar{z}$ is the expectation value of the electron distance from the interface, and a_0 is Bohr radius of the interface impurity state. The results are given with $a=b$ for (a) the GaAs/vacuum, (b) $GaAs/Ga_{1-x}Al_xAs$, (c) Si/vacuum, and (d) Si/SiO_2 interfaces. The result for a model Si interface is given (e) where all the parameters are the same as those of the Si/SiO_2 interface except the dielectric constant ϵ_2 is given by $\epsilon_1/\epsilon_2=1.2$. The solid lines correspond to $0\le a/a_0\le 5$, and the dashed lines correspond to $5\le a/a_0\le 50$. The results also apply for the case where $b\rightarrow\infty$, if the unit of the abscissa is changed from a/a_0 to $\sqrt{2}a/a_0$.

purity energy bands $E_b/|E_g^{(0)}|$ will be less than 1%. For Si/SiO_2 interfaces with a high density of interface defects ($N > 10^{12}/cm^2$), the interface condition must be taken into consideration in order to estimate the energy levels of the interface impurity states. Recent experiments and numerical calculations have shown[27–29] that because of the large lattice mismatch between Si and SiO_2, SiO_2/Si interfaces for Si with (001) orientation tend to become rough during oxidation processes even though the Si surfaces are atomically flat at the beginning of oxidation. It is suggested that SiO_2/(001)Si interfaces have Si protrusions delineated by {111} facets or similar shapes with the average height of the protrusion of 10–20 Å.[27–29] The density of interface defects calculated from the {111} facet Si-protrusion model with a height of the protrusion of 10–20 Å is $N=(1-5)\times 10^{13}$ cm^{-2}, which indicates that for these SiO_2/(001)Si interfaces, the effects of the interface defects on the interface impurity states, such as broadenings of impurity energy bands, are strong. Theoretical analysis of experimental results related with impurity states on these SiO_2/(001)Si interfaces should take interface qualities into consideration.

To estimate the effect of rough SiO_2/(001)Si interfaces on impurity states by periodically structured interfaces, we have implicitly made two approximations: (i) We have assumed that all interface defects are the same; and (ii) we have assumed that all interface defects arrange periodically on the interfaces. The first approximation is the same as that in Ref. 29 where the authors modeled rough SiO_2/(001)Si interfaces by interfaces with equal-size Si protrusions delineated by {111} facets. The second approximation may be explained as follows. Electrons in interface impurity states distribute mainly in a half-sphere centered on the impurity ions. The radius of the projected area of this half-sphere on the interface is given by $\bar{\rho}=\langle\psi_g(\mathbf{r})|\rho|\psi_g(\mathbf{r})\rangle=15\pi a_0/16\cong\pi a_0$, which for the SiO_2Si interface is about 50 Å. Only defects within this area affect dominantly the interface impurity states. Defects outside this area, whether they are periodically or randomly distributed, have little influence on the interface impurity states. For a SiO_2/Si interface with a density of interface defects N smaller than 10^{13} cm^{-2}, the average diameter of the interface defects is larger than 30 Å. Within this area, to which the electron of an interface impurity state is mainly confined, there are only a few neighboring defects. Whether these defects are distributed periodically or randomly will not appreciably change our calculated results. As commented above, the effect of rough SiO_2/(001)Si interfaces on the binding energies of impurity states obtained in our paper is expected to be smaller than that in realistic cases where interface defects, such as Si protrusions delineated by {111} facets, are much sharper than those cosine-shaped structures considered here. The results of our previous work show that a sharper interface defect causes larger shifts in the impurity state energies than those caused by a flat defect.[29]

The situation is different for the case of $GaAs/Ga_{1-x}As_xAs$ interfaces where the Bohr radius a_0 is much bigger than that of Si/SiO_2 interfaces (see Table I). Electrons in the interface impurity states will be affected by the interface structures even for structured $GaAs/Ga_{1-x}Al_xAs$ interfaces with large periods. For $GaAs/Ga_{1-x}Al_xAs$ lateral surface superlattices produced by MBE growth of AlAs/GaAs fractional-layer superlattices on [001] vicinal GaAs substrates with a period $d=100$ Å, we have $\sqrt{2}a/a_0=0.25$ (notice for one-dimensional periodically structured interfaces, the unit of the abscissa in Fig. 1 is $\sqrt{2}a/a_0$). If the height of the interface structure is $h=35$ Å, which can be realized experimentally,[19,20] we have $h/\bar{z}=0.1$, which indicates that our theory is valid. From Fig. 1(b) we have $E_b/|E_g^{(0)}|=35\%$. Interface structures will change significantly the energy levels of the interface impurity states on $GaAs/Ga_{1-x}Al_xAs$ interfaces, which may be used to design new types of electronic and optical devices.

Comparing the results of the GaAs/vacuum and $GaAs/Ga_{1-x}Al_xAs$ interfaces in Figs. 1(a) and 1(b) and Table I, we see that the effects of the interface structures on the interface impurity states increase as the dielectric constant ϵ_2 of semiconductor II approaches ϵ_1 of semiconductor I, as long as the interface can be approximated by an infinitely high potential barrier that confines the electron within semiconductor I. This is also true for the Si interfaces. In Fig. 1(e), we give the results for a model calculation where all the parameters are the same as those of the Si/SiO_2 interface, except the dielectric constant ϵ_2 of semiconductor II is taken by $\epsilon_1/\epsilon_2=1.2$. As ϵ_2 approaches ϵ_1, the effects of the interface structures are increased by the following two factors. (i) $\delta\tilde{E}_g$ increases for the same a/a_0. (ii) The Bohr radius of the interface impurity states a_0 increases, which causes the electrons in the interface impurity states to be more strongly affected by the interface structures. Though the average electron distance $\bar{z}$ from the interfaces also increases, which reduces the width of the impurity energy bands $E_b/|E_g^{(0)}|=2h|\delta\tilde{E}_g|/\bar{z}$ caused by the interface structures, the total effect is an increase of $E_b/|E_g^{(0)}|$. For instance, if we take $d=100$ Å and $h=35$ Å, from Figs. 1(a) and 1(b) we have $E_b/|E_g^{(0)}|=12\%$ for GaAs/vacuum interfaces where $\epsilon_1/\epsilon_2=12$, and $E_b/|E_g^{(0)}|=35\%$ for $GaAs/Ga_{1-x}Al_xAs$ interfaces where $\epsilon_1/\epsilon_2=1.2$. Thus, by adjusting the dielectric constants of the semiconductors forming the interfaces, the effects of the interface structures on the interface impurity states can be either reduced or increased.

ACKNOWLEDGMENT

This work was supported by the National Natural Science Foundation of China under Grant No. 19004006.

*Present address: Department of Physics and Institute of Condensed Matter Physics, Jiao Tong University, Shanghai 200030, The People's Republic of China.

[1]J. D. Levine, Phys. Rev. **140**, A586 (1965).

[2]R. J. Bell, Jr., T. Bousman, G. M. Goldman, and D. G. Rathbun, Surf. Sci. **7**, 293 (1967).

[3]B. V. Petukhov, V. L. Pokrovskii, and A. V. Chaplik, Sov. Phys. Solid. State **9**, 51 (1967).

[4]F. Stern and W. E. Howard, Phys. Rev. **163**, 816 (1967).

[5]D. Schechter, H. V. Romero, and R. J. Bell, Surf. Sci. **11**, 352 (1968).

[6]V. E. Godwin and W. E. Tefft, Surf. Sci. **34**, 108 (1973).

[7]N. O. Lipari, J. Vac. Sci. Technol. **15**, 1412 (1978).

[8]S. W. Gu and R. S. Zheng, Solid State Commun. **62**, 695 (1987); Phys. Rev. B **36**, 3280 (1987).

[9]G. Bastard, Phys. Rev. B **24**, 4714 (1981).

[10]G. Bastard, J. Lumin. **30**, 488 (1985).

[11]C. Mailhiot, Y. C. Chang, and T. C. McGill, Phys. Rev. B **26**, 4449 (1982).

[12]G. Brozak, B. D. McCombe, and D. M. Larsen, Phys. Rev. B **40**, 1265 (1989).

[13]M. Stopa and S. Das Sarma, Phys. Rev. B **40**, 8466 (1989).

[14]L. E. Oliveria and R. P. Alvarez, Phys. Rev. B **40**, 10460 (1989).

[15]H. Sakaki, K. Wagatsuma, J. Hamasaki, and S. Saito, Thin Solid Films **36**, 497 (1976).

[16]P. M. Petroff, A. C. Gossard, and W. Wiegmann, Appl. Phys. Lett. **45**, 620 (1984).

[17]A. C. Warren, D. A. Antoniadis, H. I. Smith, and J. Melngailis, IEEE Electron. Device Lett. **6**, 294 (1985).

[18]T. Fukui and H. Saito, Appl. Phys. Lett. **50**, 824 (1987).

[19]M. Tanaka and H. Sakaki, Jpn. J. Appl. Phys. **27**, L2025 (1988).

[20]M. Tsuchiya, J. M. Gaines, R. H. Yan, R. J. Simes, P. O. Holtz, L. A. Coldren, and P. M. Petroff, Phys. Rev. Lett. **62**, 466 (1989).

[21]K. Ismail, W. Chu, A. Yen, D. A. Antoniadis, and H. I. Smith, Appl. Phys. Lett. **54**, 460 (1989).

[22]H. L. Stormer, L. N. Pfeiffer, K. W. Baldwin, K. W. West, and J. Spector, Appl. Phys. Lett. **58**, 726 (1991).

[23]H. Sun and S. W. Gu, Phys. Rev. B **42**, 7556 (1990).

[24]L. I. Schiff, *Quantum Mechanics,* 3rd ed. (McGraw-Hill, New York, 1968), pp. 255–263.

[25]S. Lang, *Undergraduate Analysis* (Springer-Verlag, New York, 1983), Chap. 19.

[26]G. Beni and T. M. Rice, Phys. Rev. B **18**, 768 (1978).

[27]A. H. Carim and A. Bhattacharyya, Appl. Phys. Lett. **46**, 872 (1985).

[28]I. Ohdomari, H. Akatsu, Y. Yamakoshi, and K. Kishimoto, J. Non-Cryst. Solids **89**, 239 (1987).

[29]H. Akatsu, Y. Sumi, and I. Ohdomari, Phys. Rev. B **44**, 1616 (1991).