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LETTER TO THE EDITOR

Shallow states of donor impurities on periodically rough semiconductor interfaces

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Abstract. Ground state energies of shallow states of donor impurities on cosine-shaped periodically rough interfaces formed by two isotropic semiconductors, such as GaAs/$Ga_{1-x}Al_xAs$ or GaAs/vacuum are calculated variationally with the approximation that interfaces represent infinitely high potential barriers. The results show that changes in the ground state energies of interface impurity states caused by rough interfaces are not negligible especially for GaAs/$Ga_{1-x}Al_xAs$ interfaces with sharp defects.

Shallow states of donor impurities on semiconductor interfaces have long been the focus of extensive studies by many authors, because a number of properties of semiconductor-interface devices are strongly influenced by these impurity interface states (Levine 1965, Bell *et al* 1967, Petukhov *et al* 1967, Stern and Howard 1967, Schechter *et al* 1968, Godwin and Tefft 1973, Lipari 1978, Gu and Zheng 1987a, b). 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 were also extensively studied (Bastard 1981 and 1985, Mailhiot *et al* 1982, Brozak *et al* 1989, Stopa and DasSarma 1989, Oliveria *et al* 1989).

All these studies assumed that semiconductor interfaces are ideally planar. In realistic devices, however, it is almost impossible to fabricate ideally planar semiconductor interfaces because of environmental fluctuations and mechanical control inaccuracy in the process of device manufacturing. Deviations of semiconductor interfaces from planes will modify results predicating the energy levels of interface impurity states calculated with semiconductor interfaces assumed to be planar. In this letter, we calculate shallow states of donor impurities on periodically rough semiconductor interfaces which deviate slightly from planes. We intend to study in what way and to what extent rough interfaces will change the energy levels of interface impurity states from those calculated by assuming planar interfaces. For simplicity, we consider an interface formed by two isotropic semiconductors, such as GaAs/$Ga_{1-x}Al_xAs$ or GaAs/vacuum, with a donor impurity ion located on the interface. The results for interfaces formed by anisotropic

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semiconductors, such as Si/SiO_2, will be given elsewhere. The rough interface is assumed to be cosine shaped, and given by

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

Since by Fourier transformation, any rough interface can be considered to be the superposition of interfaces given by equation (1) with different a and b, the results of our calculation will give indications of the effects of rough interfaces on interface impurity states for general rough interfaces. For small roughness, 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. This approximation is well satisfied for the GaAs/vacuum surface and for the GaAs/$Ga_{1-x}Al_xAs$ interface with $x > 0.2$. The Hamiltonian for the interface impurity state reads

$$H = -(\hbar^2/2m_e)\nabla_r^2 + V(r) \qquad z > f(x, y) \tag{2}$$

with the electron wave function $\psi(r)$ satisfying the boundary condition

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

where we have assumed that the electron is confined within semiconductor I which occupies a space $z > f(x, y)$. The potential $V(r)$ 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, which can be obtained by solving the static Poisson equation (Sun and Gu 1990).

Up to the first order in the interface deviation from planar, the potential is given by (Sun and Gu 1990):

$$V(r) = -\frac{e^2}{\bar{\varepsilon}|r - r_i|} + Q\frac{e^2}{4\varepsilon_1 z} + Q\frac{e^2}{2\pi\varepsilon_1}\int d\rho' f(\rho')\frac{R_1(\rho' - \rho)^2 + R_2 z^2}{[(\rho' - \rho)^2 + z^2]^3}$$
$$- Q\frac{e^2}{\pi\varepsilon_1}\int d\rho' f(\rho')\frac{R_1(\rho' - \rho)\cdot(\rho' - \rho_i) + R_2 z z_i}{[(\rho' - \rho)^2 + z^2]^{3/2}[(\rho' - \rho_i)^2 + z_i^2]^{3/2}} \tag{4}$$

where ε_1 (ε_2) is the dielectric constant of semiconductor I (II). r_i is the position vector of the donor impurity on the interface, and

$$\rho = (x, y) \qquad \bar{\varepsilon} = (\varepsilon_1 + \varepsilon_2)/2 \qquad R_1 = \varepsilon_1/(\varepsilon_1 + \varepsilon_2)$$
$$R_2 = \varepsilon_2/(\varepsilon_1 + \varepsilon_2) \qquad Q = (\varepsilon_1 - \varepsilon_2)/(\varepsilon_1 + \varepsilon_2). \tag{5}$$

From the variation method (see for example, Schiff 1968), the ground state energy of the impurity state is given by the minimum of the following quantity

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

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

$$\begin{cases} \tilde{x} = x - x_i \\ \tilde{y} = y - y_i \\ \tilde{z} = z - h\cos(x/a)\cos(y/b). \end{cases} \tag{7}$$

In $\tilde{r}$ space, the rough interface $z = f(x, y)$ is transformed to a planar interface $\tilde{z} = 0$. The quantity F becomes

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

$$= \int_{-\infty}^{\infty} \mathrm{d}\tilde{x}\, \mathrm{d}\tilde{y} \int_0^{\infty} \mathrm{d}\tilde{z}\, \tilde{\psi}^*(H_{\mathrm{eff}}\tilde{\psi}). \tag{6'}$$

Where $J(\tilde{x}, \tilde{y}, \tilde{z})$ is the Jacobian determinant introduced into the integration when transforming from coordinate system (x, y, z) to $(\tilde{x}, \tilde{y}, \tilde{z})$ (see for example, Lang 1983). To obtain the last result in equation (6′), we notice that for the coordinate transformation (7), $J(\tilde{x}, \tilde{y}, \tilde{z}) = 1$, and we also require that $\tilde{\psi}$ be normalized in $\tilde{r}$ space.

$$H_{\mathrm{eff}} = H_0 + H_1 \tag{8}$$

where

$$H_0 = -(\hbar^2/2m_e)\nabla_{\tilde{r}}^2 - (e^2/\bar{\varepsilon}\tilde{r}) + Q\, e^2/4\varepsilon_1 \tilde{z} \tag{9}$$

and H_1 is a small perturbation, which is Hermitian and goes to zero when $h/\bar{z} \to 0$. The complicated expression of H_1 will be given elsewhere. In space $\tilde{r}$, the boundary condition (equation (3)) becomes

$$\tilde{\psi}|_{\tilde{z}=0} = 0. \tag{10}$$

Since H_{eff} is Hermitian, it is easy to prove (Schiff 1968) that F (equation (6′)) reaches its minimum, which is the ground state energy of the interface impurity state, when $\tilde{\psi}$ is the ground state eigenfunction of H_{eff} subject to the boundary condition (10).

In what follows, we remove the tilde on $\tilde{\psi}$ and $\tilde{r}$ to simplify the notation. But one must keep in mind that we are working in the transformed space. We expand the ground state wave function of H_{eff} (8) by hydrogenic wave functions

$$\psi_g(r) = \sum_{nlm} C_{nlm} \varphi_{nl}(r) Y_{lm}(\theta, \varphi). \tag{11}$$

To satisfy the boundary condition (10), we have $C_{nlm} = 0$ unless $m + l =$ odd integers (Levine 1965). In numerical calculations, we must cut off the infinite expansion series of $\psi_g(r)$ (11). For small roughness ($h/\bar{z} \ll 1$), where the energy shift caused by the rough interface, that is H_1 in equation (8), is much less than the level spacing between the ground and first excited states, we take

$$\psi_g(r) = C_{210}\varphi_{21}(r)Y_{10}(\theta, \varphi) = Cz \exp[-(\beta/a_0)\sqrt{\rho^2 + z^2}] \tag{12}$$

where C is the normalization constant, $a_0 = \hbar^2\bar{\varepsilon}/m_e e^2$ and β is the variational parameter introduced to compensate the interruption of the expansion series (11). The shifts in the ground state energies of the interface impurity states, $\delta\tilde{E}_g = (E_g - E_g^{(0)})/|E_g^{(0)}|(z_i/\bar{z})$, as functions of a/a_0 are calculated for the GaAs/$Ga_{1-x}Al_xAs$ interface (figure 1(a)) and GaAs/vacuum surface (figure 1(b)), where $z_i = h\cos(x_i/a)\cos(y_i/b)$ is the position of the impurity ion on the interface and $E_g^{(0)}$ are the ground state energies of interface impurity states with planar interfaces. In the calculation, we took $a = b$. The experimental parameters used are listed in table 1 together with other quantities calculated from them.

From figure 1, the following points are worth mentioning. When $z_i > 0$, the impurity ion locates on the part of the interface sunk into the semiconductor I, for the GaAs/$Ga_{1-x}Al_xAs$ interface where $\varepsilon_1/\varepsilon_2 \geq 1$, $\delta\tilde{E}_g$ is always negative. The ground state energy E_g of the interface impurity state is lower with the impurity ion on the part of the interface sunk into GaAs than with the impurity ion on the part of the interface projecting out

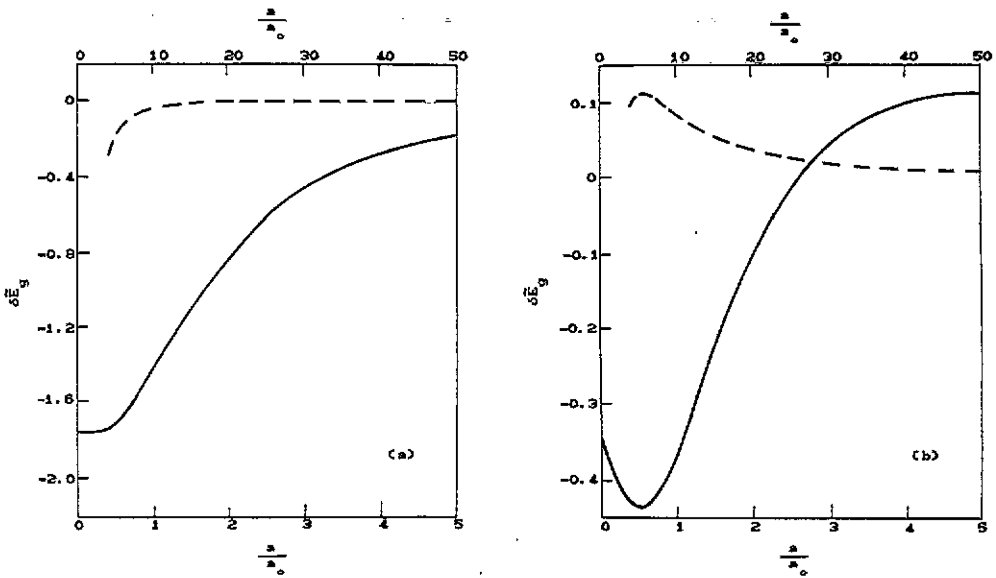

Figure 1. Shifts $\delta \tilde{E}_g$ (defined in the text) in the ground state energies of interface impurity states calculated as functions of a/a_0 for the cosine-shaped rough GaAs/$Ga_{1-x}Al_xAs$ interface (a) and GaAs/vacuum surface (b), where a is the periodicity of the rough interface and a_0 is Bohr radius of the interface impurity state defined in the text. The solid curves correspond to $0 \leq a/a_0 \leq 5$ and the broken curves correspond to $5 \leq a/a_0 \leq 50$.

Table 1. The experimental parameters used in the calculation where ε_1 and m_c are the dielectric constant and electron band mass of GaAs (Beni and Rice 1978), ε_2 is the dielectric constant of $Ga_{1-x}Al_xAs$ taken with composition $x > 0.3$ (Mailhiot *et al* 1982) to ensure the validity of the infinitely high potential barrier approximation (see the text). $E_g^{(0)}$ (in meV) is the ground state energy, $a_0 = h^2\bar{\varepsilon}/m_c e^2$ (in Å) is the Bohr radius and $\bar{z}$ (in Å) is the expectation value of the electron distance from the interface of the interface impurity state for a planar interface.

Interfaces	ε_1	ε_2	m_c	$E_g^{(0)}$	a_0	$\bar{z}$
GaAs/$Ga_{1-x}Al_xAs$	12.35	10.29	0.066	−1.644	90.77	351.4
GaAs/vacuum	12.35	1.0	0.066	−3.452	53.52	242.5

of GaAs. But for the GaAs/vacuum surface where $\varepsilon_1/\varepsilon_2 \gg 1$, $\delta \tilde{E}_g$ is negative when $a/a_0 < 2.6$ and positive when $a/a_0 > 2.6$. That is, for sharp defects ($a/a_0 \leq 1$) E_g is lowered when the impurity ion is on the part of the surface sunk into GaAs and for flat defects ($a/a_0 \gg 1$) E_g is lowered when the impurity ion is on the part of the surface projecting out of GaAs. The last result is consistent with our early calculations (Sun and Gu 1990) where we calculated the ground state energies of surface impurity states for GaAs/vacuum surfaces with certain idealized flat defects.

If impurities distribute homogeneously on interfaces, the energy levels of interface impurity states are broadened to impurity energy bands. If interactions among impurities can be neglected, the width of the impurity energy bands is given by $E_b = 2(h/\bar{z})|E_g^{(0)} \delta \tilde{E}_g|$. For a GaAs/$Ga_{1-x}Al_xAs$ interface with sharp defects, we have $E_b/|E_g^{(0)}| = 29\%$ for $h/\bar{z} = 0.1$ and $a/a_0 = 1$. Effects of rough interfaces on interface

impurity states are not negligible especially for the GaAs/$Ga_{1-x}Al_xAs$ interface with sharp defects.

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References

Bastard G 1981 *Phys. Rev.* B **24** 4714
—— 1985 *J. Lumine.* **30** 488
Bell R J, Bousman Jr T, Goldman G M and Rathbun D G 1967 *Surf. Sci.* **7** 293
Beni G and Rice T M 1978 *Phys. Rev.* B **18** 768
Brozak G, McCombe B D and Larsen D M 1989 *Phys. Rev.* B **40** 1265
Godwin V E and Tefft W E 1973 *Surf. Sci.* **34** 108
Gu S-W and Zheng R S 1987a *Solid State Commun.* **62** 695
—— 1987b *Phys. Rev.* B **36** 3280
Lang S 1983 *Undergraduate Analysis* (New York: Springer) ch 19
Levine J D 1965 *Phys. Rev.* A **140** 586
Lipari N O 1978 *J. Vac. Sci. Technol.* **15** 1412
Mailhiot C, Chang Y C and McGill T C 1982 *Phys. Rev.* B **26** 4449
Oliveria L E and Alvarez R P 1989 *Phys. Rev.* B **40** 10460
Petukhov B V, Pokrovskii V L and Chaplik A V 1967 *Sov. Phys.–Solid State* **9** 51
Schechter D, Romero H V and Bell R J 1968 *Surf. Sci.* **11** 352
Schiff L I 1968 *Quantum Mechanics* 3rd edn (New York: McGraw-Hill) pp 255–63
Stern F and Howard W E 1967 *Phys. Rev.* **163** 816
Stopa M and DasSarma S 1989 *Phys. Rev.* B **40** 8466
Sun H and Gu S-W 1990 *Phys. Rev.* B **42** unpublished