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Effects of dielectric mismatch on shallow donors and acceptors in a spherical GaAs–$Ga_{1-x}Al_xAs$ quantum dot

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Abstract. We calculate the effects of dielectric mismatch on shallow donors and acceptors in a spherical GaAs–$Al_{1-x}Ga_xAs$ quantum dot for both a finite barrier and an infinitely high barrier using the variational approach. The results have shown that the addition of dielectric mismatch enhances impurity binding energies considerably, especially when the radius of the quantum dot is small. The results also showed that the effects of dielectric mismatch on donors are comparable with those on acceptors, and the corresponding effects for an infinitely high barrier are larger than for a finite barrier.

1. Introduction

In the past few years, there has been an increasing interest in the study of quantum wells and quantum wires. With the recent advances in the art of microfabrication, it is possible to confine the carriers in all three dimensions (quantum dots or quantum boxes) [1–3]. These structures provide a great deal of new phenomena and potential device application in the future laser and optical modulation technology [4–6]. The impurity states in these quasi-zero-dimensional structures have been investigated extensively [7–10]. Zhu *et al* [7] have obtained the exact solutions of donor states in a spherical quantum dot by a numerical method, using different series forms in different regions of the radial equation. Chuu *et al* [8] have calculated the eigenenergies of an impurity in a spherical quantum dot by means of the Whittaker function and the scattering Coulomb wavefunction. Recently, Porras-Montenegro and Perez-Merchancano [9] also studied the impurity states in a quantum dot using the variational approach. The results have shown that there are stronger confinement and larger binding energy for a hydrogenic impurity in a zero-dimensional system than in the comparable two-dimensional quantum well and one-dimensional quantum wire.

Usually, the dielectric mismatch between the barrier material and well material is disregarded in studying the impurity states. In fact, the dielectric mismatch is an important factor which affects the impurity binding energies. This topic has been studied extensively by many researchers [10–21] in the low-dimensional systems, but where only the effects of dielectric mismatch on donor states are considered. Although Elabsy [17] has studied the effects of dielectric mismatch on donors and acceptors in the quantum wells, the image potential operator that he gave is incorrect. In two of our previous papers [19, 20], we have discussed the effects of dielectric mismatch on donors in the quantum wires with an infinitely high barrier, and where the effects of the electron image potential on electronic states are not considered. In another previous paper [21], the effects of electron image potential on electronic states are included in calculating the binding energies of donors in the quantum wells. The results have shown that the effects of the impurity ion image potential on impurity binding energies are much larger than those of the electron image potential, which corrected the results obtained by Elabsy [17] and those in our previous papers [19, 20]. In this paper, we investigate the effects of dielectric mismatch on the donor and acceptor states in a spherical quantum dot for both a finite barrier and an infinitely high barrier, including the impurity ion image potential only. Also, the effective-mass approximation and variational approach are used in our calculation. In section 2, we outline the theoretical framework. The results and discussion are presented in section 3.

2. Theory

When an impurity ion with a positive charge e is placed at the centre of a GaAs quantum dot with a $Ga_{1-x}Al_xAs$ barrier, the following expression can be obtained by means of electrodynamics

$$\iint \boldsymbol{D} \cdot \mathrm{d}\boldsymbol{S} = 4\pi e \tag{1}$$

where

$$\boldsymbol{D} = \epsilon \boldsymbol{E} \tag{2}$$

is the vector of electric displacement. The electric field is given by

$$E = \frac{e}{\epsilon r^2}. \tag{3}$$

The impurity potentials inside and outside the quantum dot are as follows:

$$V(r) = -\int_{\infty}^{r} -\frac{e^2}{\epsilon r^2}\,\mathrm{d}r = \begin{cases} -\dfrac{e^2}{\epsilon_1 r} + \dfrac{e^2}{\epsilon_1 R_0} - \dfrac{e^2}{\epsilon_2 R_0} & r \leqslant R_0 \\ -\dfrac{e^2}{\epsilon_2 r} & r \geqslant R_0 \end{cases} \tag{4}$$

where R_0 is the radius of quantum dot, and

$$\epsilon_1 = 13.1\epsilon_0 \tag{5a}$$

$$\epsilon_2 = [13.1(1-x) + 10.1x]\epsilon_0 \tag{5b}$$

are the static dielectric constants for GaAs and $Ga_{1-x}Al_xAs$, respectively [15], with ϵ_0 the vacuum static dielectric constant. The contributions of dielectric mismatch to the impurity potential inside and outside the quantum dot are obtained:

$$V_1(r) = \begin{cases} \left(\dfrac{1}{\epsilon_1} - \dfrac{1}{\epsilon_2}\right)\dfrac{e^2}{R_0} & r \leqslant R_0 \\ \left(\dfrac{1}{\epsilon_1} - \dfrac{1}{\epsilon_2}\right)\dfrac{e^2}{r} & r \geqslant R_0. \end{cases} \tag{6}$$

The Hamiltonian of the hydrogenic impurity in the spherical quantum dot can be written

$$H(\boldsymbol{r}) = \begin{cases} \dfrac{|\boldsymbol{P}|^2}{2m_1} & \qquad r \leqslant R_0 \\ & +V(\boldsymbol{r}) \\ \dfrac{|\boldsymbol{P}|^2}{2m_2} + V_0 & \qquad r \geqslant R_0 \end{cases} \tag{7}$$

where m_1 and m_2 are the electron-band effective masses in GaAs and $Ga_{1-x}Al_xAs$, respectively, and V_0 is the electron-confining potential in the quantum dot, which is equal to the conduction or valence band discontinuity between the barrier material and the well material. Since the alloy composition range that we studied was such that the alloy was direct ($x < 0.45$), both the effective mass m_2 and the conduction or valence band offset V_0 were determined [15, 17] using the $\boldsymbol{k} = \boldsymbol{0}$ values in $Ga_{1-x}Al_xAs$, i.e. we take

$$m_1 = 0.067m_0 \tag{8a}$$

$$m_2 = (0.067 + 0.083x)m_0 \tag{8b}$$

$$V_0 = 0.6\Delta E_g^{\Gamma}(x) \tag{8c}$$

for the conduction band, and

$$m_1 = m_2 = 0.30m_0 \tag{9a}$$

$$V_0 = 0.4\Delta E_g^{\Gamma}(x) \tag{9b}$$

for the valence band with mixing of the light- and heavy-hole bands neglected [22], where m_0 is the free-electron mass and $\Delta E_g^{\Gamma}(x)$ is the difference between the $Ga_{1-x}Al_xAs$ and GaAs band gaps at the Γ point, which is given by [23]

$$\Delta E_g^{\Gamma}(x) = 1.155x + 0.37x^2 \text{ eV}. \tag{10}$$

As in [9], the ground electronic wavefunctions of the Hamiltonian in the absence of the impurity are as follows:

$$\phi_{10}(r) = N_0 \begin{cases} \dfrac{\sin(\xi_{10}r)}{r} & r \leqslant R_0 \\ \dfrac{\sin(\xi_{10}R_0)}{r}\exp[\chi_{10}(R_0 - r)] & r \geqslant R_0 \end{cases} \tag{11}$$

where N_0 is the normalization constant, and the parameters

$$\xi_{10} = (2m_1E_{10}/\hbar^2)^{1/2} \tag{12a}$$

$$\chi_{10} = [2m_2(V_0 - E_{10})/\hbar^2]^{1/2}. \tag{12b}$$

The ground-state electronic level E_{10} is determined using the appropriate current-conserving boundary conditions for the wavefunctions at the interfaces and must satisfy the following relation:

$$-\xi_{10} = \left[\frac{m_1}{m_2}\chi_{10} - \left(1 - \frac{m_1}{m_2}\right) \Big/ R_0\right]\tan(\xi_{10}R_0). \tag{13}$$

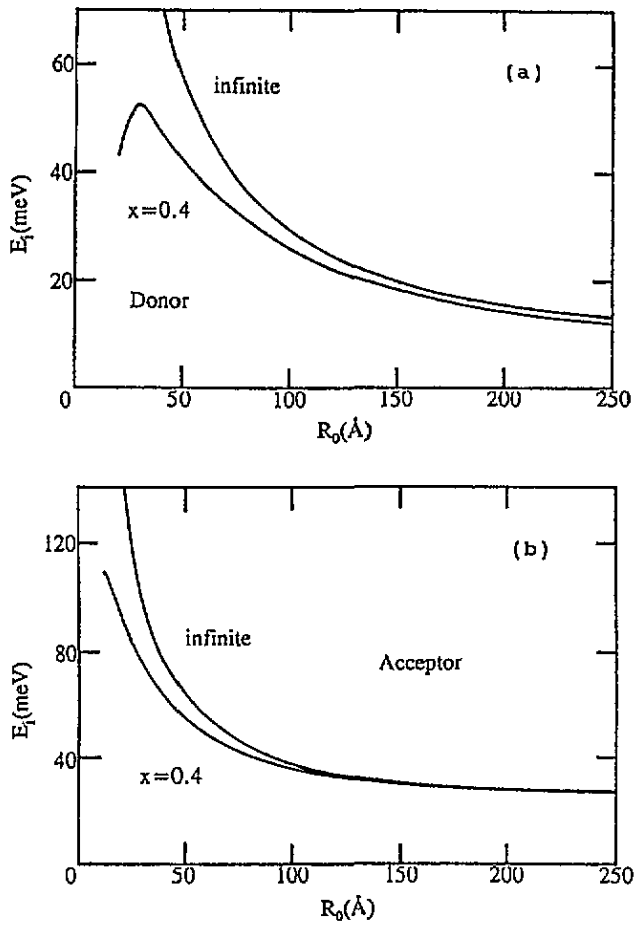

Figure 1. Variations in impurity binding energy with the radius of quantum dot for $x = 0.4$ and an infinitely high barrier, where the impurity is placed at the centre of the quantum dot: (*a*) donor; (*b*) acceptor.

The smallest radius for the existence of a bound state can be obtained from equation (13):

$$R_0 = \left[\frac{\pi^2\hbar^2}{8m_1V_0} + \frac{\hbar^2}{2m_2V_0}\left(\frac{m_2}{m_1} - 1\right)^2\right]^{1/2}. \qquad (14)$$

The trial wavefunction of $H(r)$ that we take is analogous to that used in [9] and is written for the ground impurity state as

$$\phi(r) = N\phi_{10}(r)\exp(-r/\lambda) \qquad (15)$$

where N is the normalization constant and λ is the variational parameter.

As usual, the impurity binding energy is defined as the energy difference between the bottom of the electronic energy band without the impurity and the ground-state level of the impurity state in the quantum dot, i.e.

$$E_i = E_{10} - \min_{\lambda}\langle\phi(r)|H(r)|\phi(r)\rangle. \qquad (16)$$

The above integrals were calculated numerically.

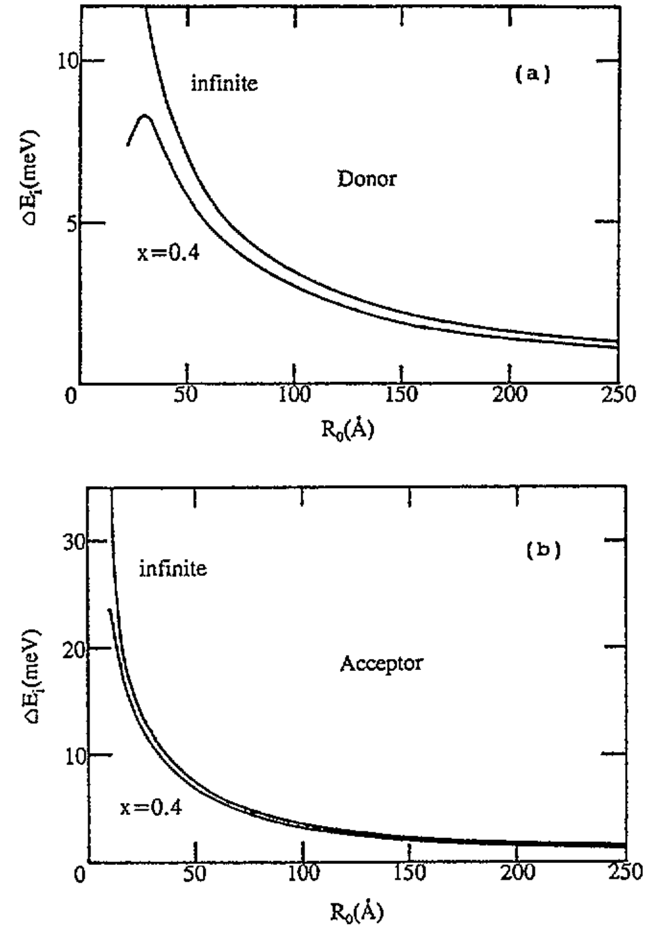

Figure 2. Variations in the differences between the impurity binding energies of the cases including and excluding the dielectric mismatch with the radius of the quantum dot for $x = 0.4$ and an infinitely high barrier, where the impurity is placed at the centre of the quantum dot: (*a*) donor; (*b*) acceptor.

3. Results and discussion

In this paper, the two cases of infinitely high confining potential and $x = 0.4$ for the barrier material are considered. The impurity binding energies for donors and acceptors in the spherical quantum dot excluding dielectric mismatch obtained by us agree well with the results in [9] as shown in figure 1, where $\epsilon_1 = \epsilon_2 = 13.1\epsilon_0$ and $m_1 = m_2 = m$ with m the electron band effective mass in GaAs.

From figure 2, it is apparent that, when the dielectric mismatch is included, the impurity binding energies change markedly, especially when the radius of quantum dot is small. In figure 2, we can also see that the effects of dielectric mismatch on impurity states for an infinitely high barrier are larger than those for $x = 0.4$. For an infinitely high barrier, when the radius R_0 of the quantum dot is 250 Å, the difference ΔE_i between the impurity binding energies of the cases including and excluding the dielectric mismatch is 1.36 meV for donors and acceptors; when the radius R_0 of quantum dot is reduced to 30 Å, the corresponding

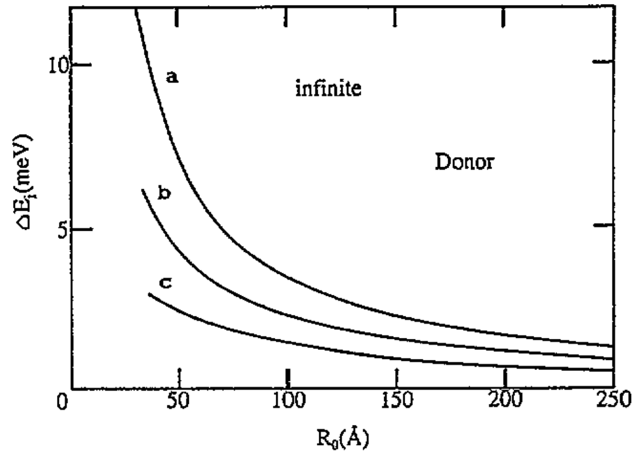

Figure 3. The differences between the binding energies of the cases including and excluding the impurity ion image potential for donors and an infinitely high barrier in the spherical quantum dot (curve a) in the square quantum wire (curve b) (taken from [19,20]) and in the quantum well (curve c) (taken from [21]), where the widths of square quantum wire and quantum well are $2R_0$ and the impurity is placed at the centre of the quantum dot, quantum wire and quantum well.

difference ΔE_i is 11.33 meV for donors and acceptors. For $x = 0.4$, when the radius R_0 of the quantum dot equals 250 Å, the differences ΔE_i between the impurity binding energies of the cases including and excluding the dielectric mismatch are 1.21 meV and 1.20 meV for donors and acceptors, respectively; when the radius R_0 of the quantum dot is reduced to 30 Å, the corresponding differences ΔE_i are 8.33 meV and 9.88 meV for donors and acceptors, respectively. These indicate that the effects of dielectric mismatch on donors are comparable with those on acceptors in the quantum dot. However, the peak of the difference ΔE_i with $x = 0.4$ for acceptors is much higher than that for donors, as shown in figure 2. In addition, our results also indicate that the effects of dielectric mismatch on impurity binding energies in the quantum dots are larger than those in the quantum wells [21] and quantum wires [16, 19, 20], as shown in figure 3.

In conclusion, we have calculated the effects of dielectric mismatch on donors and acceptors in the spherical GaAs–$Ga_{1-x}Al_xAs$ quantum dot for both a finite barrier and an infinitely high barrier. From equation (6), it can be easily seen that the contributions of dielectric mismatch to the impurity potential inside and outside the quantum dot are negative, which have the same sign as that of the impurity potential, and the contribution of dielectric mismatch to the impurity potential inside the quantum dot increases with decrease in the radius of the quantum dot apparently; so the dielectric mismatch enhances the impurity binding energies considerably, especially when the radius of the quantum dot becomes small. In fact, the effects of dielectric mismatch on donors and acceptors are the same for an infinite barrier, which are equal to the first branch of equation (6) analytically, and the effects of dielectric mismatch on donors are comparable with those on acceptors in the spherical quantum dot. Because of the heavier effective mass and smaller effective Bohr radius for holes ($m_h = 0.3m_0$; $a^* = 22$ Å) than for electrons ($m_e = 0.067m_0$; $a^* = 100$ Å) in GaAs, the peak of the difference ΔE_i between the impurity binding energies of the cases including and excluding the dielectric mismatch with $x = 0.4$ for acceptors is higher than that for donors. The results also showed that the effects of dielectric mismatch on impurity binding energies for an infinitely high barrier are larger than for $x = 0.4$ owing to the stronger confinement of electron in the quantum dot with an infinitely high confining potential.

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