Impurity states in a spherical GaAs-$Ga_{1-x}Al_xAs$ quantum dot: Effects of the spatial variation of dielectric screening

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We calculate the binding energies of 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, including the spatial variation of dielectric screening. The results show that when the spatial variation of dielectric screening is considered, the impurity binding energies increase noticeably, especially when the radius of the quantum dot is small. The results also show that the effects of spatial variation of dielectric screening on acceptors are larger than those on donors. The dielectric mismatch in this structure is also discussed.

I. INTRODUCTION

Recent developments in the art of microfabrication have made it possible to confine the carriers in all three dimensions (quantum dots or quantum boxes).[1-3] These structures may create many new phenomena and they show great potential for device applications in the future in laser and optical-modulation technology.[4-6] The impurity states in these quasi-zero-dimensional structures have been investigated extensively.[7-9] Zhu, Xiang, and Gu[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, Hsiao, and Mei[8] have calculated the eigenenergies of an impurity in a spherical quantum dot by means of the Whittaker function and scattering Coulomb wave function. Recently, Porras-Montenegro and Perez-Merchancano[9] studied the impurity states in a quantum dot using the variational approach. The results showed that there is a stronger confinement and a larger binding energy for a hydrogenic impurity in a zero-dimensional system than those in the comparable two-dimensional quantum well and one-dimensional quantum wire.

However, the spatially dependent screening of an impurity ion caused by the valence electrons and the dielectric mismatch between the barrier material and well material are usually disregarded. These topics have been discussed by many researchers[10-23] for the quantum wells and quantum wires but, where the spatial variation of dielectric screening or the dielectric mismatch is considered independently, they found that the spatial variation of dielectric screening and the dielectric mismatch are important. In this paper, we investigate the donor and acceptor states in a spherical quantum dot for both finite barrier and infinitely high barrier, including the spatial variation of dielectric screening. The dielectric mismatch in this structure is also included. In our previous papers,[22,23] the results have shown that the effects of impurity ion image potential due to dielectric mismatch on impurity binding energies are much larger than those of electron image potential, and only the impurity ion image potential is considered in this study. Also, the effective-mass approximation and variational approach are used in our calculation. In Sec. II, we outline the theoretical framework. Results and discussion are presented in Sec. III.

II. THEORY

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

$$\int\int \mathbf{D}\cdot d\mathbf{S}=4\pi e \ , \tag{1}$$

where

$$\mathbf{D}=\epsilon(r)\mathbf{E} \tag{2}$$

is the vector of electric displacement. If the dielectric function is assumed to be a spherical symmetry, the electric field is given by

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

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

$$V(\mathbf{r})=-\int_{\infty}^{r}-\frac{e^2}{\epsilon(r)r^2}dr$$
$$=\begin{cases}-\dfrac{e^2}{\epsilon_1(r)r}+\dfrac{e^2}{\epsilon_1(R_0)R_0}-\dfrac{e^2}{\epsilon_2(R_0)R_0}, & r\le R_0\\ -\dfrac{e^2}{\epsilon_2(r)r}, & r\ge R_0,\end{cases} \tag{4}$$

where R_0 is the radius of the quantum dot. The form of dielectric response adopted in this paper is the same as that proposed by Hermanson,[24]

$$\epsilon_1^{-1}(r)=\epsilon_1^{-1}+(1-\epsilon_1^{-1})\exp(-r/\alpha)\ , \tag{5a}$$
$$\epsilon_2^{-1}(r)=\epsilon_2^{-1}+(1-\epsilon_2^{-1})\exp(-r/\alpha)\ , \tag{5b}$$

where $\alpha=1.1$ a.u. is the screening parameter,[11–13] and

$$\epsilon_1=13.1\epsilon_0 \tag{6a}$$
$$\epsilon_2=[13.1(1-x)+10.1x]\epsilon_0 \tag{6b}$$

are the static dielectric constants for GaAs and $Ga_{1-x}Al_xAs$, respectively,[18] with ϵ_0 the vacuum static dielectric constant. Here, $\epsilon_1(r)$ and $\epsilon_2(r)$ are substantially different from $\epsilon(r)$.

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

$$H(\mathbf{r})=\begin{cases}\dfrac{\mathbf{p}^2}{2m_1}+V(\mathbf{r}), & r\le R_0\\ \dfrac{\mathbf{p}^2}{2m_2}+V_0+V(\mathbf{r}), & r\ge R_0,\end{cases} \tag{7}$$

where m_1 and m_2 are the electron-band effective mass in the GaAs and $Ga_{1-x}Al_xAs$; 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 well material. Since the alloy composition range 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[18,20] using the $\mathbf{k}=0$ values in $Ga_{1-x}Al_xAs$, that is, 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 conduction band, and

$$m_1=m_2=0.30m_0 \tag{9a}$$
$$V_0=0.4\Delta E_g^{\Gamma}(x) \tag{9b}$$

for valence band with the mixing of the light- and heavy-hole bands neglected,[25] 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[26]

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

As in Ref. 9, the ground electronic wave functions of the Hamiltonian in the absence of the impurity are as follows:

$$\phi_{10}(r)=N_0\times\begin{cases}\dfrac{\sin(\xi_{10}r)}{r}, & r\le R_0\\ \dfrac{\sin(\xi_{10}R_0)}{r}e^{\chi_{10}(R_0-r)}, & r\ge R_0\ ,\end{cases} \tag{11}$$

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 electronic level E_{10} is determined by using the appropriate current-conserving boundary conditions for the wave functions at the interfaces. It must satisfy the following relation:

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

The smallest radius for the existence of a bound state can be obtained from Eq. (13),

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

The trial wave function of $H(\mathbf{r})$ that we take is analogous to that used in Ref. 9 and is written for the ground impurity state as

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

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 conduction band without the impurity and the ground level of the impurity state in the quantum dot, that is

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

The above integrals were calculated numerically.

III. RESULTS AND DISCUSSION

In this paper, the two cases of infinitely high confining potential and composition $x=0.4$ for the barrier material are considered. The impurity binding energies for donors and acceptors in the spherical quantum dot, excluding the spatial variation of dielectric screening obtained by us, agree well with the results in Ref. 9, as shown in Fig. 1. The impurity states including the spatial variation of dielectric screening and neglecting the dielectric mismatch are also discussed, as shown in Fig. 2, where $\epsilon_1=\epsilon_2=13.1\epsilon_0$ and $m_1=m_2=m$ with m the electron-band effective mass in the GaAs.

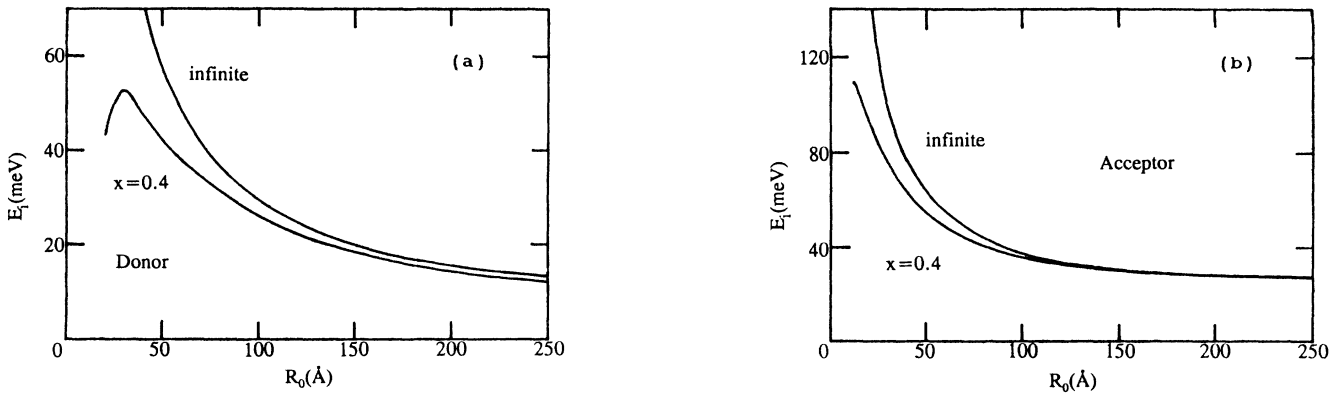

FIG. 1. Variations in impurity binding energy with the radius of the quantum dot for composition $x=0.4$ and infinitely high barrier, where the impurity is placed at the center of the quantum dot. (a) Donor. (b) Acceptor.

From Fig. 2, it is apparent that when the spatial variation of dielectric screening is included, the impurity binding energies change markedly, especially when the radius of the quantum dot is small. In Fig. 2, we can also see that the effects of spatial variation of dielectric screening on impurity states for infinitely high barrier are much larger than those for composition $x=0.4$, and the corresponding effects on acceptors are larger than those on donors. For infinitely high barriers, when the radius of the quantum dot is $R_0=250$ Å, the differences ΔE_i between the impurity binding energies of the cases including and excluding the spatial variation of dielectric screening are nearly zero and 1.56 meV for donor and acceptor, respectively, which tend to the corresponding values in the bulk GaAs; when the radius of the quantum dot is reduced to $R_0=20$ Å for the donor and $R_0=15$ Å for the acceptor, the corresponding differences ΔE_i reach 5.89 and 36.66 meV for donor and acceptor, respectively. For composition $x=0.4$, when the radius of the quantum dot is $R_0=250$ Å, the differences ΔE_i between the impurity binding energies of the cases including and excluding the spatial variation of dielectric screening are nearly the same as those for the infinitely high barrier; when the radius of quantum dot is reduced to $R_0=20$ Å for the donor and $R_0=10$ Å for the acceptor, the corresponding differences ΔE_i are 2.03 and 13.34 meV for the donor and acceptor, respectively. In addition, our results indicate that the effects of spatial variation of dielectric screening on impurity binding energy in the quantum dots are larger than those in the quantum wells[10] and quantum wires.[11–13]

Figure 3 shows the difference between the impurity binding energies including and excluding the spatial variation of dielectric screening, where the dielectric mismatch between the barrier material and well material is also considered. Comparing the results in Fig. 2, we can easily see that the spatial variation of dielectric screening enhances impurity binding energies more apparently in Fig. 3, especially when the radius of the quantum dot is small, and the effects of dielectric mismatch on impurity states is important. Also, the corresponding effects for an infinitely high barrier are much larger than those for composition $x=0.4$. For an infinitely high barrier, when the radius of the quantum dot is $R_0=250$ Å, the differences ΔE_i between the impurity binding energies of the cases including and excluding the spatial variation of dielectric screening are 1.67 and 2.86 meV for the donor and acceptor, respectively; when the radius of the quantum dot is reduced to $R_0=30$ Å for the donor and $R_0=20$ Å for the acceptor, the corresponding differences ΔE_i reach 15.61 and 35.98 meV for the donor and acceptor, respectively. For composition $x=0.4$,

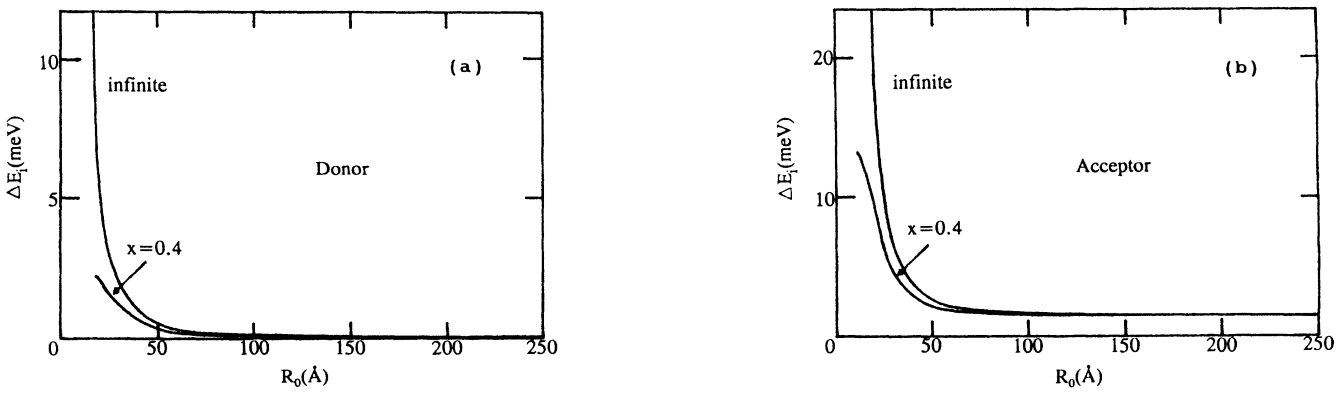

FIG. 2. Variations in the differences between the impurity binding energies of the cases including and excluding the spatial variation of dielectric screening with the radius of the quantum dot for composition $x=0.4$ and infinitely high barrier, where the impurity is placed at the center of the quantum dot. (a) Donor. (b) Acceptor.

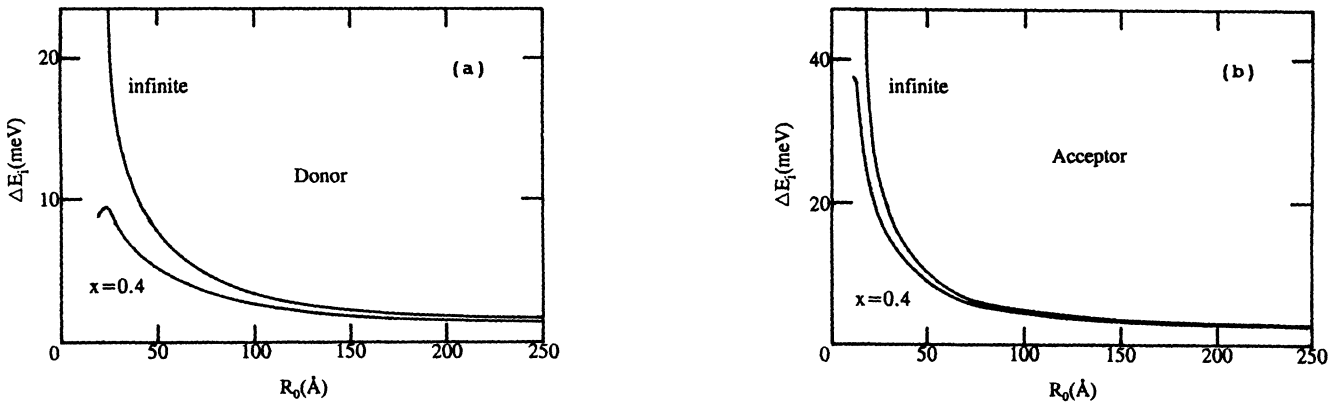

FIG. 3. Variations in the differences between the impurity binding energies of the cases including and excluding the spatial variation of dielectric screening with the radius of the quantum dot for composition $x=0.4$ and infinitely high barrier, where the dielectric mismatch is also considered and the impurity is placed at the center of the quantum dot. (a) Donor. (b) Acceptor.

when the radius of the quantum dot is $R_0=250$ Å, the differences ΔE_i between the impurity binding energies of the cases including and excluding the spatial variation of dielectric screening are 1.33 and 2.67 meV for the donor and acceptor, respectively; when the radius of the quantum dot is reduced to $R_0=20$ Å for the donor and $R_0=10$ Å for the acceptor, the corresponding differences ΔE_i are 9.41 and 37.83 meV for the donor and acceptor, respectively.

Summing up, we have calculated the effects of spatial variation of dielectric screening on impurity binding energies in a spherical GaAs-$Ga_{1-x}Al_xAs$ quantum dot for both a finite barrier and an infinitely high barrier. The results show that the spatial variation of dielectric screening enhances the impurity binding energies considerably, especially when the radius of the quantum dot becomes small, and the dielectric mismatch between the barrier material and well material is also important. Because of the heavier effective mass and smaller effective Bohr radius for the hole ($m_h=0.3m_0$, $a^*=22$ Å) than those for the electron ($m_e=0.067m_0$, $a^*=100$ Å) in the GaAs, the effects of spatial variation of dielectric screening on acceptors are larger than those on donors. The results also show that the effects of spatial variation of dielectric screening on impurity binding energies for an infinitely high barrier are much larger than those for composition $x=0.4$ due to the stronger confinement of electron in the quantum dot with infinitely high confining potential.

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