The influence of compressive stress on shallow-donor impurity states in symmetric GaAs-$Ga_{1-x}Al_xAs$ double quantum dots

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The effects of compressive stress on the binding energy of shallow-donor impurity states in symmetrical GaAs-$Ga_{1-x}Al_xAs$ double quantum dots are calculated variationally using a parameterized wave function within the effective-mass approximation. Results are obtained for different dot and barrier widths, donor ion positions, and compressive stresses along the growth direction of the structure. In the direct-gap regime (for stress values up to 13.5 kbar) the binding energy increases linearly with the stress. In the indirect-gap regime (for stress values greater than 13.5 kbar) and with the donor ion at the center of the dot, the binding energy increases up to a maximum and then decreases. For all donor ion positions, the binding energy shows nonlinear behavior in the indirect-gap regime due to the Γ-X crossing effect. In the limit of single quantum wells, the results we obtain are in good agreement with those previously obtained for the case in which the donor ion is at the center of the well. © *2007 American Institute of Physics*.
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I. INTRODUCTION

Since the pioneering work by Bastard on the donor impurity binding energy in quantum wells,[1] much effort has been devoted to this subject.[2–7] Particular attention has been given to the effects of the reduction of dimensionality, changes in the cross-sectional geometry, applied electric and magnetic fields, and uniaxial stress applied to semiconductor heterostructures. Theoretical work related to the Seffects of hydrostatic pressure and compressive stress on shallow-donor impurity states in GaAs-$Ga_{1-x}Al_xAs$ quantum wells has been reported over the last ten years.[8–11] These authors have considered Γ-X crossover and, as a general feature, have found a linear dependence of the binding energy on the applied pressure in the direct-gap regime, while in the indirect-gap regime (applied pressure larger than 13.5 kbar) the energy grows with the pressure until reaching a maximum and then decreases. In addition, they have shown a red-shift in the shallow-donor-related optical-absorption spectra associated with the pressure dependence of the semiconductor band gap.

The optical properties associated with shallow-donor impurities in multiple GaAs-$Ga_{1-x}Al_xAs$ quantum well structures are of interest due to their potential applications in optoelectronics. This is due in part to the fact that it is possible, by applying external pressures, to modulate both the absorption spectra from states in the valence band and the emission spectra from states in the conduction band. In both cases the final states are related to randomly distributed donor impurities along the structure.

Using the masked implantation enhanced intermixing technique and the dry etching technique with subsequent overgrowth, Schweizer *et al.*[12] realized rectangular cross section GaAs-$Ga_{1-x}Al_xAs$ quantum-well wires and quantum dots, allowing the effects of stress on low-dimensional heterostructures to be studied experimentally. Oyoko *et al.*[13] studied the effects of a uniaxial stress on the binding energy of a shallow donor impurity in a parallelepiped-shaped GaAs-$Ga_{1-x}Al_xAs$ quantum dot. In the calculations, they used a variational technique within the effective-mass approximation, but did not consider the effects of electron tunneling or electron effective-mass mismatch.

As far as we know, no studies have been made of stress effects on the binding energies of shallow donor impurities in symmetrical GaAs-$Ga_{1-x}Al_xAs$ double quantum dots (DQDs). In the present paper, using the effective-mass approximation and the variational method, we present theoretical calculations of the effects of an external compressive stress on the binding energy of shallow donor impurities in symmetrical GaAs-$Ga_{1-x}Al_xAs$ DQDs structures. The effects of dot and barrier width and donor ion position are all taken into account. Image charge effects, however, are not considered. The work is organized as follows: In Sec. II we present our theoretical framework; in Sec. III we give our results and discussion, and finally in Sec. IV we present our conclusions.

II. THEORETICAL FRAMEWORK

In the effective-mass approximation, the Hamiltonian for a hydrogenic shallow-donor impurity in symmetrical GaAs-$Ga_{1-x}Al_xAs$ DQDs including the effects of temperature (T) and a compressive stress (P) in the x direction is given by

$$H = -\frac{\hbar^2}{2m^*_{d,b}(P,T)}\nabla^2 - \frac{e^2}{\varepsilon_{d,b}(P,T)r} + V(x,y,z,P,T), \qquad (1)$$

where $r=\sqrt{(x-x_i)^2+y^2+z^2}$ is the distance between the electron and the donor ion, and subscripts d and b stand for the quantum dot and the barrier layer materials, respectively. $(x_i,0,0)$ is the donor ion position. $m^*_{d,b}$ are the conduction

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effective masses of the quantum dot and the barrier layer materials as functions of P and T,[14]

$$m_d^*(P,T) = \left[1 + 7.51\left(\frac{2}{E_g(P,T)} + \frac{1}{E_g(P,T)+0.341}\right)\right]^{-1} m_0, \tag{2}$$

where m_0 is the free-electron mass. $E_g(P,T)$ is the stress-dependent band gap for the GaAs semiconductor at the Γ point and at low temperatures, and can be expressed as[15]

$$E_g(P,T) = 1.519 + 10.7 \times 10^{-3}P - 5.405 \times 10^{-4}T^2/(T+204). \tag{3}$$

The barrier effective mass depends on the aluminum concentration (x) as

$$m_b^* = m_d^* + 0.083 x m_0. \tag{4}$$

$\varepsilon_{d,b}(P,T)$ are the static dielectric constants of the quantum dot and the barrier layer materials. At $T=4$ K the stress-dependent GaAs static dielectric constant is given by[16]

$$\varepsilon_d(P,4\text{ K}) = 12.83\exp(-1.67 \times 10^{-3}P). \tag{5}$$

The dielectric constant mismatch between ε_b and ε_d affects the binding energy mainly for small quantum dot widths and high aluminum concentrations.[9] Strictly speaking, the image potential in DQDs cannot be neglected when considering electronic and impurity states, especially when the sizes of the dots are small. However, in our calculations we use an aluminum concentration of $x=0.3$, and the structures are generally of a large size. Due to the fact that in the present work we focus our attention on stress effects, charge image effects have not been considered. This means that in the Hamiltonian of Eq. (1) $\varepsilon_b(P,T)=\varepsilon_d(P,T)$.[17]

$V(x,y,z,P,T)$ is the potential that confines the electron in the quantum dot, and is given by

$$V(x,y,z,P,T) = \begin{cases} V_0(P,T), & \text{for } |x| \le L_b/2 \text{ with } |y| < L_y/2 \text{ and } |z| < L_z/2, \\ 0, & \text{for } L_b/2 < |x| < L_c \text{ with } |y| < L_y/2 \text{ and } |z| < L_z/2, \\ V_0(P,T), & \text{for } |x| \ge L_c \text{ with } |y| < L_y/2 \text{ and } |z| < L_z/2, \\ \infty, & \text{otherwise}, \end{cases} \tag{6}$$

where $L_c(P)=L_b/2+L_d$, and L_b and L_d are the stress-dependent widths in the x direction of the central barrier layer and of a single quantum dot, respectively. $V_0(P,T)$ is the stress-dependent barrier height.[18–21] L_y and L_z give the dimensions of the DQDs in the other two directions. L_b and L_c can be obtained by the fractional change in volume, which for a zinc-blend crystal of volume V is given by[17]

$$\frac{\delta V}{V} = -3P(S_{11}+S_{12}), \tag{7}$$

where $S_{11}=1.16\times10^{-3}$ kbar^{-1} and $S_{12}=-3.7\times10^{-4}$ kbar^{-1} are the elastic constants of GaAs.[22]

For computational purposes, we normalize the above expression in energy units of the electron Rydberg constant, $R_y=e^2/2a_B\varepsilon$, where $a_B=\hbar^2\varepsilon/e^2m_e^*$ is the electron Bohr radius and m_e^* is the electron effective mass in GaAs bulk materials for $P=0$.

In symmetrical GaAs-$Ga_{1-x}Al_xAs$ DQDs, the Hamiltonian for an electron is

$$H = -\frac{1}{\alpha}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(x,y,z,P,T), \tag{8}$$

where α is m_d^*/m_e^* in GaAs and m_b^*/m_e^* in GaAs-$Ga_{1-x}Al_xAs$, respectively. The value of α can be obtained from Eqs. (2) and (4).

The ground-state energy of an electron in symmetrical GaAs-$Ga_{1-x}Al_xAs$ DQDs can be expressed as

$$E_0^e(P,T) = E_0^x(P,T) + E_0^y + E_0^z, \tag{9}$$

where $E_0^y=(\pi/L_y)^2$ and $E_0^z=(\pi/L_z)^2$ are the ground-state energies along the y and z directions, respectively. The eigenfunction can be written in the following separated form:

$$f(x,y,z) = \begin{cases} h(x)\cos(\pi y/L_y)\cos(\pi z/L_z), & \text{for } |y| < L_y/2 \text{ and } |z| < L_z/2 \\ 0, & \text{otherwise} \end{cases}. \tag{10}$$

Here $h(x)$ is the eigenfunction along the x direction

$$h(x)=\begin{cases} A\exp[k_2(x+L_c)], & \text{for } x\le -L_c \\ -B\sin[k_1(x+L_b/2)]+C\cos[k_1(x+L_b/2)], & \text{for } -L_c<x<-L_b/2 \\ [\exp(k_2x)+\exp(-k_2x)]/2, & \text{for } |x|\le L_b/2 \\ -B\sin[k_1(x-L_b/2)]+C\cos[k_1(x-L_b/2)], & \text{for } L_b/2<x<L_c \\ A\exp[-k_2(x-L_c)], & \text{for } x\ge L_c \end{cases}, \tag{11}$$

where

$$k_1=\sqrt{E_0^x(P,T)},\quad k_2=\sqrt{V_0(P,T)-E_0^x(P,T)}. \tag{12}$$

The coefficients A, B, and C are obtained from the boundary conditions of the eigenfunction $h(x)$ at the interfaces $x=\pm L_c$ and $x=\pm L_b/2$.

The corresponding eigenvalue associated with $h(x)$, $E_0^x(P,T)$, may be obtained as the first root of the transcendental equation

$$2\cos(k_1L_d)+\left(\beta-\frac{1}{\beta}\right)\sin(k_1L_d) -\left(\beta+\frac{1}{\beta}\right)\sin(k_1L_d)\exp(-k_2L_b)=0, \tag{13}$$

where $\beta=m_d^*k_2/m_b^*k_1$.

Within the variational procedure, the trial wave function for the ground state of the shallow-donor impurity in symmetrical GaAs-$Ga_{1-x}Al_xAs$ DQDs can be written as

$$\psi(r)=Nf(x,y,z)g(r), \tag{14}$$

where

$$g(r)=\exp(-\lambda r) \tag{15}$$

is the hydrogenic part; λ is a variational parameter, and N is the normalization constant.

The compressive stress dependence of the impurity binding energy is calculated from the definition

$$E_b(P,T)=E_0^e(P,T)-E_{\min}(P,T), \tag{16}$$

where $E_{\min}(P,T)$ is the eigenvalue of the Hamiltonian in Eq. (1), minimized with respect to the variational parameter λ.

In the next section, all of the results are for a symmetrical GaAs-$Ga_{0.7}Al_{0.3}As$ DQD and are for an assumed temperature of $T=4$ K.

III. RESULTS AND DISCUSSION

In Fig. 1, we present results for the binding energy of a shallow-donor impurity in a symmetrical GaAs-$Ga_{1-x}Al_xAs$ DQD as a function of the donor ion position along the x direction, considering different values of the applied compressive stress. When the donor ion position goes from the center of the barrier to the center of the right dot, the binding energy increases gradually and reaches a maximum value at the center of the right dot. Then, when the donor ion moves toward the dot edge, the binding energy decreases but is larger at the edge of the dot than at the edge of the barrier. This is due to the stronger confinement of the barrier. When the donor ion is located at the center of the barrier, the binding energy increases with decreasing barrier width for a given value of the stress. However, as observed, in the region of the dot there is a crossing between the corresponding solid and dashed curves, at a constant applied stress, because the binding energy increases faster with increasing barrier width, which is equivalent to a higher confinement.

In Fig. 2 we show the binding energy as a function of the dot width $L_d(L_y=L_z=L_b=200$ Å) for four different positions of the donor ion: At the barrier center, at the barrier edge, at the dot center, and at the dot edge. The binding energy increases with increasing dot width for small dot sizes, reaches a maximum value corresponding to the distance between the donor ion and the electron reaching its minimum value (see Fig. 3), and finally decreases monotonically for wider dots due to the weakness of the geometric confinement. Comparing the two curves labeled 3 to the other ones, when the donor ion is located at the dot center, the binding energy is larger and influenced only weakly by the width of the dots. This is due to the fact that the electron is confined to just one dot space. Since it has less freedom to move, the average distance between the donor ion and the electron remains almost constant. This can be understood by noting that in positions 1, 2, and 4 the electron cloud has more space to distribute itself. For the curves labeled 3, when the dot sizes are

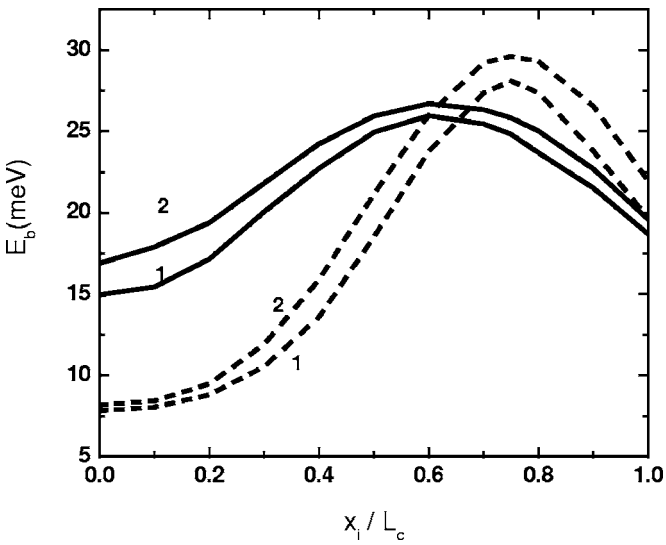

FIG. 1. Binding energy of a donor impurity as a function of the growth direction donor ion position in symmetrical GaAs-$Ga_{1-x}Al_xAs$ DQDs. The sizes of the two structures considered are $L_y=L_z=200$ Å, $L_d=100$ Å, and $L_b=50$ Å (solid lines) and $L_y=L_z=200$ Å, $L_d=100$ Å, and $L_b=200$ Å (dashed lines). Different values of the applied compressive stress, 10 kbar (1) and 30 kbar (2), are considered.

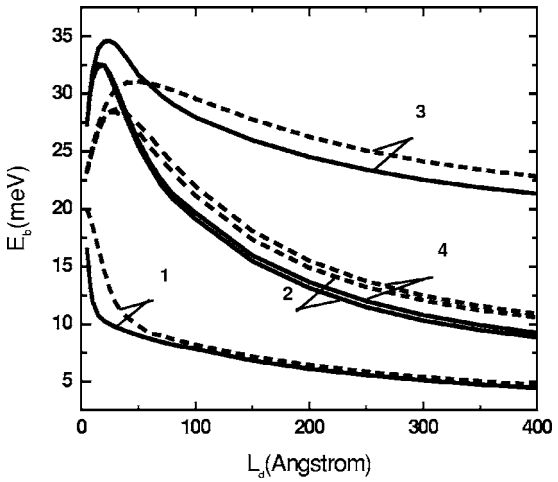

FIG. 2. Binding energy of a donor impurity as a function of the width of the dots in symmetrical GaAs-$Ga_{1-x}Al_xAs$ DQDs with $L_y=L_z=L_b=200$ Å, for $P=10$ kbar (solid lines) and $P=30$ kbar (dashed lines). The numbers 1, 2, 3, and 4 correspond to donor ions located at the barrier center, barrier edge, dot center, and dot edge, respectively.

small ($L_d<50$ Å), for $P=30$ kbar the electron is not effectively confined in the right dot, which makes the coupling of the two dots stronger than that for $P=10$ kbar. Consequently, the penetration of the electron wave function into the second dot increases and the binding energy decreases. In Fig. 3, the behavior of the average distance is seen to be the reverse of that for the binding energy. It is worth noting the change in the form of the binding energy for the two curves labeled (a), due to the strong confinement of the electron cloud at small values of L_d. For the case of large applied stress, shown by the dashed curve (a), a decrease in barrier width causes a reduction in confinement. The variation of the expectation value for $|r|$ confirms the above discussion. It should be recalled that we neglected image charge effects in the present calculations, and that consequently there may be important changes in Figs. 2 and 3 for dot widths smaller than about 50 Å when these effects are included.

The effects of the central barrier width on the binding energies for several donor ion positions and two values of the

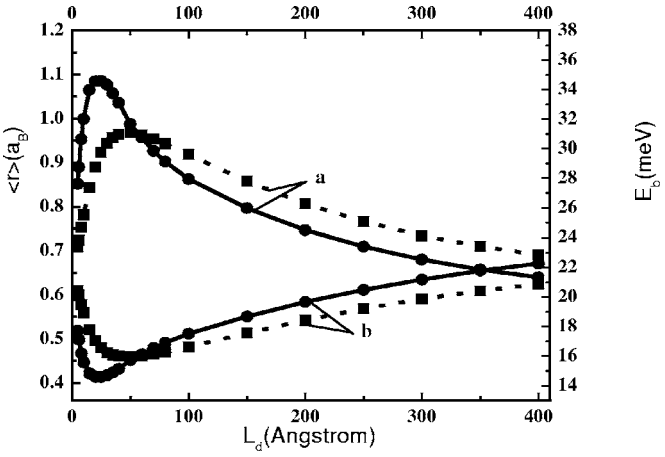

FIG. 3. Binding energy (a) and expectation value of r (b) are shown as functions of the dot width in symmetrical GaAs-$Ga_{1-x}Al_xAs$ DQDs with $L_y=L_z=L_b=200$ Å, for $P=10$ kbar (solid lines) and $P=30$ kbar (dashed lines) for the case in which the donor ion is located at the dot center.

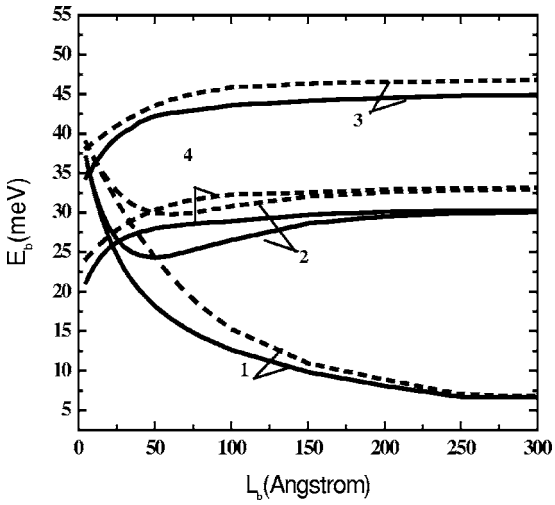

FIG. 4. Binding energy of a donor impurity as a function of the width of the central barrier in symmetrical GaAs-$Ga_{1-x}Al_xAs$ DQDs with $L_y=L_z=L_d=100$ Å, for $P=10$ kbar (solid lines) and $P=30$ kbar (dashed lines). The numbers 1, 2, 3, and 4 are the same as those in Fig. 2.

applied compressive stress are displayed in Fig. 4. When the barrier width goes to zero, the binding energy goes to the exact values for a single quantum dot with $L_d=200$ Å and $L_y=L_z=100$ Å. On the other hand, in the limit of large barrier widths, the binding energy tends to the result for decoupled quantum dots with $L_d=L_y=L_z=100$ Å. The binding energy always decreases monotonically with increasing barrier width when the donor ion is at the center of the barrier (curves labeled 1). In the L_b infinite limit, the binding energy will always go to zero because the expectation value of the distance between the donor ion and the electron goes to infinity and, therefore, the Coulomb interaction goes to zero. It is clear that for $L_b<20$ Å, the two curves labeled 1 should have almost the same binding energy value, and similarly for the curves labeled 2. This is due to the fact that the influence of the positional difference of the donor ion at the barrier center and at the barrier edge on the binding energy is very small for narrow barrier widths. It is worth noting the change in the curves labeled 2. As the barrier width increases, the binding energy of the impurity state diminishes until a minimum value is obtained. It then rises gradually and coincides with the curves labeled 4. The merging of curves 2 and 4 is the limiting case of a single quantum dot for a sufficiently large barrier width. It is clear that for ions at the center and at the edge of a dot, the coupling of the quantum dots becomes evident for L_b less than 150 Å.

The binding energy of a donor impurity as a function of the applied compressive stress in symmetrical GaAs-$Ga_{1-x}Al_xAs$ DQDs for two different values of the dot and barrier widths is presented in Fig. 5. As can be seen, for stress values up to 13.5 kbar the binding energy increases linearly with stress. This is due to the increasing barrier and electron dot effective masses as well as to the decreasing dielectric constants. For stress values higher than 13.5 kbar it is well-known that the Γ-X crossover shows up in GaAs, diminishing the barrier height with stress and causing the observed variation in the binding energy. It is important to remark that for stress values around 37 kbar there is a

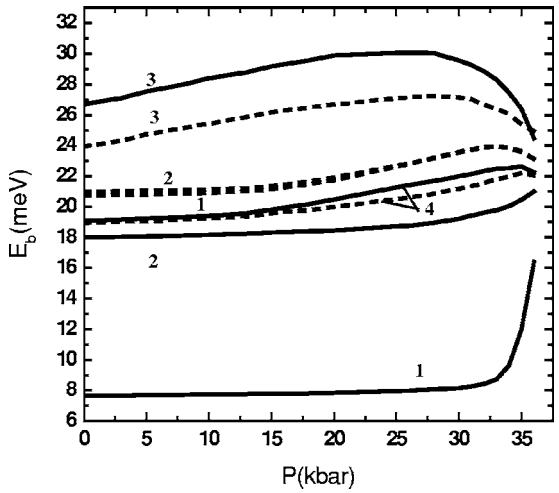

FIG. 5. Binding energy of a donor impurity as a function of the applied compressive stress in symmetrical GaAs-$Ga_{1-x}Al_xAs$ DQDs with $L_y=L_z=200$ Å and $L_d=L_b=100$ Å (solid lines) and $L_y=L_z=100$ Å, $L_d=75$ Å, and $L_b=25$ Å (dashed lines). The numbers 1, 2, 3, and 4 are the same as those in Fig. 2.

semiconductor-metal transition. For small barrier widths, the binding energy shows a softer variation, since for low stress the charge distribution is more concentrated around the donor ion. As the stress increases, the barrier height diminishes and the wave function penetrates into the central barrier. A decrease in the expectation value of the distance between the electron and the donor ion is, therefore, found resulting in an increase in the binding energy.

In Fig. 6 we contrast the binding energy of the donor impurity as a function of the applied compressive stress in symmetrical GaAs-$Ga_{1-x}Al_xAs$ DQDs for $L_y=L_z=3000$ Å, $L_d=200$ Å, and $L_b=500$ Å with that in a single quantum well when the donor ion is located at the center of the right dot.[8,9] Due to the large values of L_b, L_y, and L_z considered here, the structure is practically at the limiting case of a single quantum dot. We can observe that the binding energy reaches a maximum value for $P=26$ kbar, which is in excellent agreement with the values of Refs. 8 and 9.

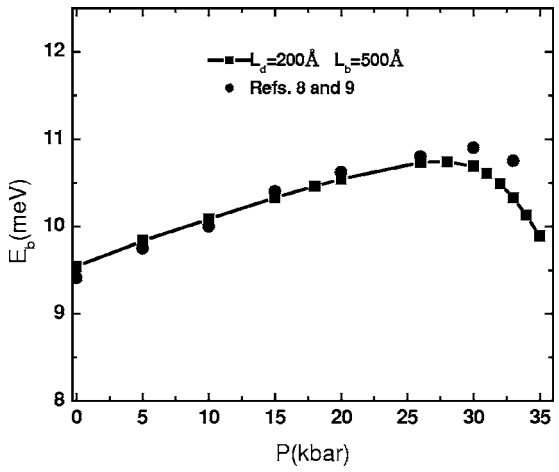

FIG. 6. Comparison of results for the binding energy in symmetrical GaAs-$Ga_{1-x}Al_xAs$ DQDs for $L_y=L_z=3000$ Å, $L_d=200$ Å, and $L_b=500$ Å with these for a single quantum well as obtained in Refs. 8 and 9. The donor ion is located at the center of the right dot.

IV. CONCLUSIONS

Theoretical calculations related to the influence of compressive stress on shallow-donor impurity states in symmetrical GaAs-$Ga_{1-x}Al_xAs$ DQDs have been presented. The main conclusions are as follows:

The effects of quantum dot size on the binding energy of donor impurity states are in good agreement with those found in previous work, both experimental and theoretical. Due to the coupling of two symmetrical GaAs-$Ga_{1-x}Al_xAs$ DQDs, we find that our results for the binding energies are all smaller than those for a single quantum dot.

By calculating the effects of the barrier width on the binding energy, we find that in the limit of large barrier width the binding energy converges to values for a single quantum dot. In addition, the binding energy of the donor ion at the barrier edge increases until the barrier becomes sufficiently large to impede wave function penetration toward the second dot. The binding energy then takes on its smallest value.

The binding energy of the donor impurity as a function of the donor ion position has also been discussed. The binding energy is much larger when the donor ion is located at the dot center than at other positions. This is because when the ion is in this position, the wave function is reduced at the boundaries and the contributions to the energy are smaller than otherwise.

We have observed that the average distance between the donor ion and the electron decreases for small quantum dot sizes, until it reaches a minimal value, and then increases with increasing quantum dot size as expected on the basis of the weakness of the geometric confinement. Consequently, the binding energy of a donor impurity is reduced as the average distance increases.

The compressive stress dependence of the binding energy for different donor ion positions in symmetrical GaAs-$Ga_{1-x}Al_xAs$ DQDs is also presented. For stress values up to 13.5 kbar, the binding energy increases linearly with the stress. For stress values greater than 13.5 kbar, the direct-gap regime passes into the indirect-gap regime, where the Γ-X crossover in GaAs reduces the barrier height with increasing stress, causing the nonlinear variation observed in the binding energy for all donor ion positions.

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