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Binding Energies of Donor States in GaAs-GaAlAs Quantum Wells Under Hydrostatic Pressure

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Abstract: The binding energies of donor states (1s, 2s, $2p_x$, $3p_x$) in GaAs-$Ga_{0.7}Al_{0.3}As$ quantum wells are investigated with a variational method under hydrostatic pressure. In the calculation, we take into account the electronic effective mass, dielectric constant and conduction band offset between the well and barriers varying with pressure. Results obtained show that the donor binding energy variation with the well width and the position of impurity under pressure is similar to that without pressure. Also the donor binding energy increases linearly with pressure for all of states in direct gap regime.

Key words: Binding energy, variational method, (1s, 2s, $2p_x$, $3p_x$) donor states, direct gap

INTRODUCTION

The binding energy of a hydrogenic impurity with in an infinite well has received much attention in Quantum Well (QW) systems (Bastard, 1981; Fraizzoli *et al*., 1990; Ferreyra and Proetto, 1991; Cen and Bajaj, 1992; Chaudhuri and Bajaj, 1994; Redinski and Janko, 2005). Similar studies (Porras-Montenegero and Perez-Marchancano, 1992, Porras-Montenegero *et al*., 1993; Ban and Liang, 2001; Aktas *et al*., 2005) have been extended for structures with lower dimensionality such as Quantum Well Wires (QWW), Quantum Dots (QD) and also for various geometries. For a number of reasons, most of the studies on these semiconductor systems have been carried out on III-V semiconductor heterostructure systems and in particular, in GaAs-$Ga_{1-x}Al_xAs$ semiconductor systems. We emphasize that the optical properties of these heterostructure systems are of significant importance for device applications and in this sense, impurity states play a relevant role. It is well known that Coulomb-bound states may be significantly modified by quantum confinement, applied external fields and hydrostatic pressure and much more experimental and theoretical studies have been devoted to the understanding of the physical properties of impurity in low-dimensional semiconductor heterostructures (Morales *et al*., 2002, 2003; Lopez *et al*., 2003a, b; Oyoko *et al*., 2001; Correa *et al*., 2004; Adachi, 1985; Beneditctal *et al*., 1993).

Effects of hydrostatic pressure modify the semiconductor band structure and lead to shift effectively the energy levels without altering the crystal symmetry of these heterostructure systems also the masses of carriers, the height barriers of the heterostructures and the Γ-X band crossover on the ground state as well as of some low lying excited states are affected by hydrostatic pressure (Elabsy, 1994; Raigoza *et al*., 2005; Neethiulagarajan and Balasubramanian, 1993; Nithiananthi and Jayakumar, 2006).

In this study, the hydrostatic pressure dependence of the ground state 1s and the 2s-, $2p_x$-, $3p_x$- like states of a shallow-donor in GaAs-$Ga_{0.7}Al_{0.3}As$ QW with finite barriers are calculated using a variational procedure with in the effective mass approximation. Results are calculated for different well widths, shallow-donor positions and hydrostatic pressure. The pressure effects of the electron effective mass, the dielectric constant and band offsets between the well and barrier materials are considered in calculations by restricting ourselves to range of pressure where there is no Γ-X crossover.

MATERIALS AND METHODS

Theoretical framework: In the effective-mass approximation, the Hamiltonian for a hydrogenic shallow donor impurity in a single GaAs-$G_{1-x}Al_xAs$ semiconductor QW under the effect of a hydrostatic pressure (P) and the temperature (T) is given by (Lopez *et al*., 2005).

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

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Where, r (= $[x^2+y^2+ (z-z_i)^2]^{1/2}$ is the carrier impurity distance and subscripts w and b stand for the quantum well layer and barrier layer materials, respectively. The pressure dependent potential energy V (z, T, P), which confines the donor electron in the well layer regions, is given by:

$$V(z,T,P) = \begin{cases} 0 & |z| < \frac{L(P)}{2} \\ V_0(P,T) & |z| \geq \frac{L(P)}{2} \end{cases} \quad (2)$$

Where, V_0 (P, T) is the pressure dependent barrier height (Elabsy, 1994) and the pressure dependent width of well layer L (P), can be obtained by using of fractional changes in volume of the structure (Kasapoglu *et al.*, 2005):

$$L(P) = L(0)[1 - (S_{11} - 2S_{12})P] \quad (3)$$

Where, S_{11} (= 1.16×10^{-3} $kbar^{-1}$) and S_{12} (= -3.7×10^{-4} $kbar^{-1}$) are the elastic constants of the GaAs (Elabsy, 1994) and L(0) is the original width of the electron confinement potentials in the z-direction without hydrostatic pressure. In Eq. 1, z_i is the impurity position with respect to the well center that it is chosen as the coordinate origin. The parabolic conduction effective-masses $m^*_{w,b}$ are given by (Elabsy, 1994)

$$m_w^*(P,T) = [1 + 7.51(\frac{2}{E_g(P,T)} + \frac{1}{E_g(P,T) + 0.341})]^{-1} m_0, \quad (4)$$

$$m_b^*(P,T,x) = m_w^*(P,T) + 0.083\, x\, m_0, \quad (5)$$

Where, m_0 is free-electron mass. In Eq. 2, E_g (P,T) is the pressure dependent energy band gap for the GaAs semiconductor at the Γ point and at low temperature. This is given by Elabsy (1994):

$$E_g(P,T) = [1.519 + 10.7\times10^{-3} - 5.405\times10^{-4}\frac{T^2}{T+204}] \quad eV. \quad (6)$$

We want to emphasize that for single quantum wells larger than 50 Å, the nonparabolic effective mass effects are lower than 5% (Chaudhuri and Bajaj, 1994). In the above expression $\varepsilon_{w,b}$ (P,T) are the corresponding static dielectric constants of well layer and barrier layer, where at T = 4 K, the GaAs static dielectric constant with respect to pressure is given by Lopez *et al.* (2005)

$$\varepsilon_w(P, 4\ K) = 12.83 \exp(-1.67\times10^{-3} P) \quad (7)$$

In present calculations we use x = 0.3 and due to the fact that the binding energy changes occur for small well width and high aluminum concentration (Elabsy, 1992), the image potential in QWs can be neglected and the charge image effects have not been considered. This means that in the Hamiltonian in Eq. 1, we take ε_w (P,T) = ε_b (P,T) (Duque *et al.*, 1997).

We use a variational approach for the calculation of the binding energies (Elabsy, 1994; Bastard, 1988) and the trial envelope wave functions $\Psi_{nl}(\vec{r})$ are thus taken as products of the hydrogenic functions Γ_{nl}, of the nth state and with *l* symmetry, with the ground state wave functions of the quantum well f(z) (Carneiro *et al.*, 1995):

$$\Psi_{nl}(\vec{r}) = N_{nl}\Gamma_{nl}(\rho, z, z_i; \lambda) f(z), \quad (8)$$

Where, N_{nl} are the normalization constants and f(z) obtained via the Hamiltonian of Eq. 1, without the impurity term. The hydrogenic variational wave functions are taken as:

$$\Gamma_{1s} = \exp(-r/\lambda_{1s}), \quad (9)$$

$$\Gamma_{2s} = (1 - \beta_{2s} r)\exp(-r/\lambda_{2s}), \quad (10)$$

$$\Gamma_{2p_x} = \rho\cos\phi\exp(-r/\lambda_{2p_x}), \quad (11)$$

$$\Gamma_{3p_x} = (2 - \beta_{3p_x} r)\rho\cos\phi\exp(-r/\lambda_{3p_x}), \quad (12)$$

Where, r = $[\rho^2 + (z-z_i)^2]^{1/2}$ and $\{\lambda_{nl}, \beta_{nl}\}$ are variational parameters obtained in such a way that E_{nl} (P,T) = $\langle\Psi_{nl}|H|\Psi_{nl}\rangle/\langle\Psi_{nl}|\Psi_{nl}\rangle$ is minimized, with the requirement that Γ_{nl} form a set of orthogonal functions (Carneiro *et al.*, 1995).

The hydrostatic pressure dependent donor binding energy is calculated as:

$$E_b(P,T) = E_0(P,T) - E_{nl}(P,T), \quad (13)$$

Where, E_0 (P,T) is the electron ground state energy without donor.

RESULTS AND DISCUSSION

Figure 1 shows the binding energies of a donor impurity for ground state and 2s-, $2p_x$-, $3p_x$-like hydrogenic excited states, as a function of quantum well widths, for on-center and on-edge donors in a GaAs-$Ga_{0.7}Al_{0.3}As$ QW, for two given pressures, p = 0 and 10 kbar. It can be observed that the binding energy increases with the applied pressure for all of states and the binding energy of a donor on-center is more than of a donor on-edge. This fact is true for all of states and result for the ground

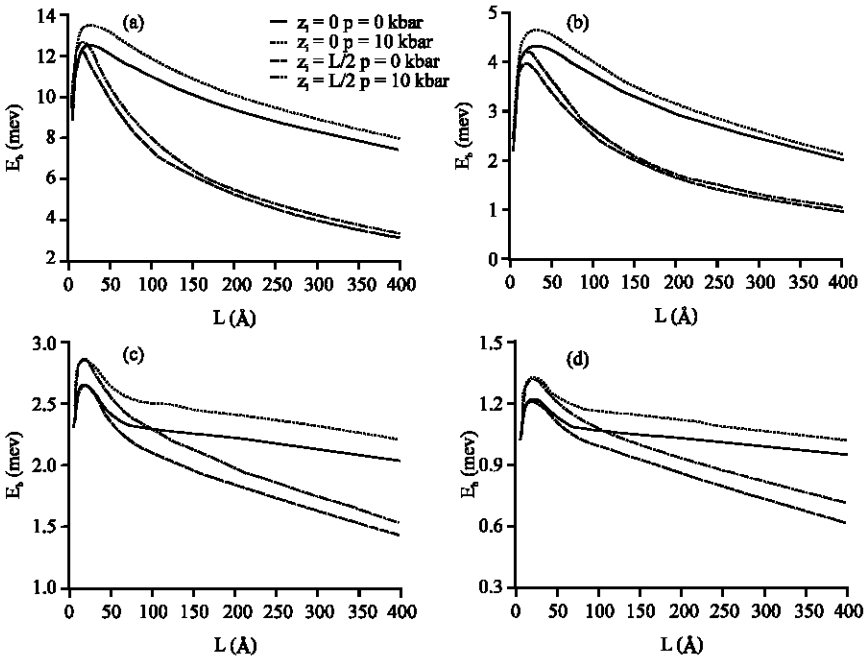

Fig. 1: Binding energies of (a) 1s, (b) 2s, (c) $2p_z$, (d) $3p_z$ like donor states as functions of the GaAs-$Ga_{0.7}Al_{0.3}As$ QW width for donor on-center and on-edge with p = 0, 10 kbar

state is in agreement with reported by Zhao *et al.* (2003). This increment of the binding energy reflects the geometrical confinement due to effective diminishing of the well width and the height of the barrier due to the applied pressure. In Fig. 1, it is shown that the two curves of the donor binding energy versus width, both on-center and on-edge, for pressure p = 0 and 10 kbar are almost parallel. One can see that the pressure effects for different pressures are qualitatively similar. Therefore, that the character of the binding energy variation with the well width under pressure is similar to that without pressure is expected.

When the well width is much larger than the effective Bohr radii of the well, the electronic wave function almost does not penetrate into the barriers and the donor binding energy decreases with increasing the well width and finally ($L\rightarrow\infty$) tends to the GaAs bulk limit. With decreasing the well width, the size of the quantum confinement in z-direction reduces and the donor binding energy increases, however, for finite barriers, the electronic wave function cannot be confined completely in the well and partly penetrates into the barriers when the well width is getting narrower than the effective Bohr radii of impurity state.

Thus, because of competition between this quantum confinement and donor energy, the donor binding energies variation with well width, are non monotonic.

Figure 2 shows our theoretical results for the binding energies of the 1s-, 2s-, $2p_z$-, $3p_z$-like donor states for GaAs-$Ga_{0.7}Al_{0.3}As$ QW as function of impurity position along the growth direction in a QW with 210 Å in width and two different pressure p = 0 and 10 kbar. The donor binding energy firstly increases and then decreases with moving the impurity position from z_i = -L to z_i = +L. The maximum binding energy is obtained for impurity located at the center of QW. It is obvious that the donor binding energy decreases when the distance of donor from the well center increases. As the pressure increase, the well width and dielectric constant decrease, the effective mass of electron increases, leading to more confinement in the well in z-direction of the impurity electron and so the donor binding energy increase for all impurity positions. The binding energy for the impurity positions closed to the barriers is lower than for on-center, since Coulomb interaction between the electron and impurity decreases. We note that for donors located at the well center, the binding energy deference between two different pressure p = 0 and 10 kbar, is more than donors located at the well edge. In other word, the hydrostatic pressure raises the binding energy mainly for on-center impurity than for on-edge ones. This result for the ground state is in good agreement with that reported by Lopez *et al.* (2005). The combined effects of hydrostatic pressure and the impurity position are really not so simple, in particular for

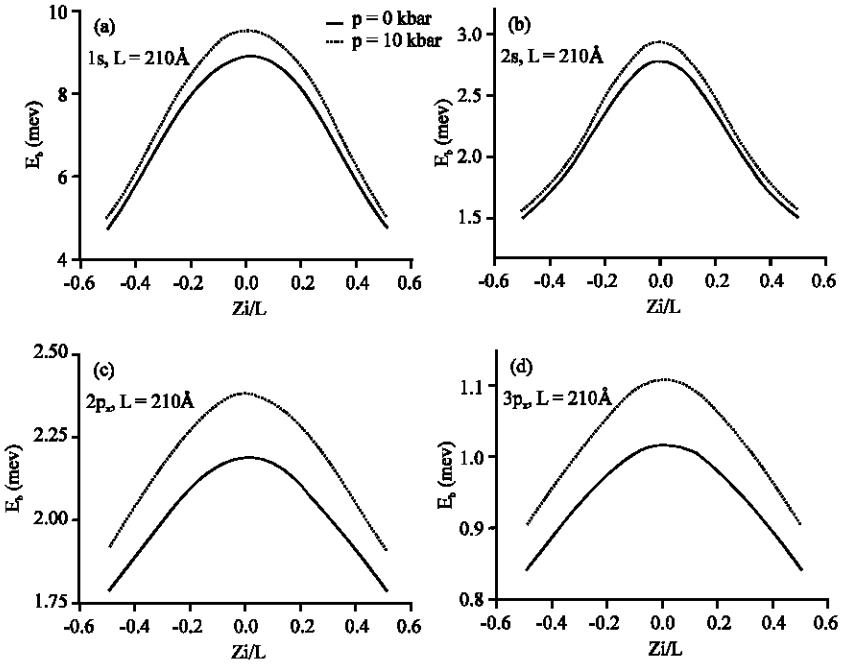

Fig. 2: Binding energy of a donor as a function of the growth-direction impurity position in GaAs-$Ga_{0.7}Al_{0.3}As$ QW with p = 0, 10 kbar for (a) 1s, (b) 2s, (c) $2p_x$, (d) $3p_x$ donor states

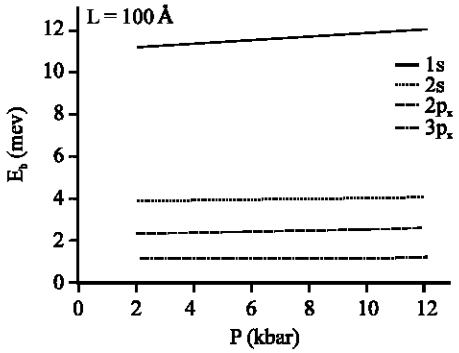

Fig. 3: Binding energies of 1s, 2s, $2p_x$, $3p_x$ like donor states in a GaAs-$Ga_{0.7}Al_{0.3}As$ QW as functions of pressure for L = 100 Å and donor in center

higher pressures (indirect gap regime), the rate at which the binding energy increases is lower and bend down to smaller values. One can see this result for other well widths in Fig. 1.

In Fig. 3 one may notice that, for pressure up to 13.5 kbar (direct gap regime), the donor binding energy increases linearly with pressure for ground state (Lopez *et al*., 2005) and excited states. This is due to the increment of the barrier and well effective mass as well as to the decrease of the dielectric constant with pressure, in other word, in this pressure regime, the Γ-X crossover for $Ga_{1-x}Al_xAs$ layer is not considered and as a consequence the barrier height that confines the electrons in GaAs layer remains constant. Also the increasing rate of binding energy with pressure for all excited states is less than 1s like state.

CONCLUSION

We have studied theoretically the effects of the applied hydrostatic pressure on the ground state and 2s, $2p_x$, $3p_x$, excited states donor binding energy in a GaAs-$Ga_{0.7}Al_{0.3}As$ single quantum well using a variational scheme within the effective mass approximation. The results show that the donor binding energy increase almost linearly with the pressure in direct gap regime and the binding energy variation with pressure for 2s, $2p_x$, $3p_x$, excited states is similar to ground state. We observe that the donor binding energy variation for all of states with the width, both for donor on-center and on-edge, are almost parallel for two different pressure and the pressure effects are qualitatively similar. We have also shown that the donor binding energy, without pressure, decreases for all of states when the distance of donor from the well center increases, furthermore for donors located at the well center, the donor binding energy deference between two different pressure, is more than the donors located at well edge.

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