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The effects of pressure and barrier height on donor binding energy in GaAs/$Ga_{1-x}Al_xAs$ cylindrical quantum well wires

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ABSTRACT

The ground state binding energy of axial hydrogenic impurity in GaAs/$Ga_{1-x}Al_xAs$ cylindrical quantum well wires (CQWWs) are investigated as a function of the barrier height and the radius of the wire under hydrostatic pressure in the effective mass approximation and variational calculation scheme. The effect of applied hydrostatic pressure is introduced into the calculations using pressure dependent values of energy gap, effective mass and dielectric constant. We have found that for large radii the binding energies are not affected by applied pressure. However, in the region where the particles interact with the barrier the binding energy is strongly dependent on the hydrostatic pressure for all x values. Furthermore, we have shown that this dependency is as strong as the binding energy increase via Al concentration increase.

1. Introduction

The physics of low-dimensional semiconductor systems such as quantum wells (QWs) [1–4], quantum wires (QWWs) [5–9] and quantum dots (QDs) [10,11] have been widely investigated in the last few decades. The study of the impurity states in these systems is important because they play crucial role in their thermal, optical and electrical properties and they can change the properties of the electronic and optoelectronic devices dramatically.

By varying the external fields, hydrostatic pressure and temperature, one can change a number of physical properties of these systems. Many studies about the effects of electric and magnetic fields binding energy calculations of hydrogenic impurities in QWs have been extensively studied [12–16].

Also, several theoretical studies about the hydrostatic pressure effects on the impurity states in low dimensional systems have been performed [17–21]. Elabsy has calculated the hydrostatic pressure dependence of the binding energy of donor in QWs and he found that the binding energy increases with increase in external hydrostatic pressure for a given quantum well thickness [17]. Correa et al. [20] have calculated the effects of hydrostatic pressure on the binding energy and the donor-related photo-ionization cross-section in 1D and 0D GaAs low dimensional systems.

In this study, we used a finite confinement potential model and variational methods in the effective mass approximation scheme; in addition we have calculated the binding energy of a shallow donor impurity in cylindrical GaAs/$Ga_{1-x}Al_xAs$ QWWs under hydrostatic pressure for a constant temperature and for $x=0.1$, 0.3 and 0.4 values. Here we follow Elabsy's model [17] in which the Γ–X crossover in the barrier material, ($Ga_{1-x}Al_xAs$)-induced by the effect of hydrostatic pressure, is introduced into the model through the pressure dependence of the height of the barrier that confines the electrons. Even though from Ref. [22] we know that for pressure values below $\approx$ 13.5 kbar (1.35 GPa) the height of the barrier remains constant, we still used Elabsy's approach since we have worked with high pressure values.

2. Theory

The Hamiltonian for a hydrogenic donor impurity in a GaAs/$Ga_{1-x}Al_xAs$ CQWW under the influence of hydrostatic pressure can be written as

$$H = H_0 - \frac{e^2}{\varepsilon(P)|\mathbf{r}-\mathbf{r}_0|} \quad (1)$$

where P is the hydrostatic pressure, $|\mathbf{r}-\mathbf{r}_0| = [\rho^2+\rho_0^2 - 2\rho\rho_0\cos(\varphi-\varphi_0)+(z-z_0)^2]^{1/2}$, $\mathbf{r}$ and $\mathbf{r}_0$ are the electron and impurity ion positions, respectively. $\varepsilon(P)$ is the dielectric constant with respect to pressure P (GPa) for GaAs. $\varepsilon(P)$ is given as follows [23]:

$$\varepsilon(P) = 13.13 - 0.088P \quad (2)$$

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For an impurity ion located at the wire axis, we take $\rho_0=0$ and $z_0=0$, which also simplifies the algebra.

Hamiltonian without Coulombic interaction is H_0 and can be written as

$$H_0=\frac{\mathbf{p}^2}{2m^*(P)}+V(\rho,P) \tag{3}$$

where $m^*(P)$ is the effective mass of an electron in GaAs as a function of hydrostatic pressure. $m^*(P)$ is determined from the expression

$$m^*(P)=m^*(0)e^{0.078P} \tag{4}$$

The total band gap (in eV units) difference between GaAs and $Ga_{1-x}Al_xAs$ as a function of x (mole fraction of aluminum) and P is given by

$$\Delta E_g(x,P)=\Delta E_g(x)+PD(x) \tag{5}$$

where $\Delta E_g(x)$ is the variation of the energy gap difference and $D(x)$ is the pressure coefficient. These variables are defined as follows for GaAs/$Ga_{1-x}Al_xAs$ system:

$$\Delta E_g(x)=1.155x+0.37x^2\,\text{eV} \tag{6}$$

$$D(x)=[-(1.3\times10^{-3})x]\,\text{eV/kbar} \tag{7}$$

The confinement potential is given by

$$V(\rho,P)=\begin{cases}0, & \rho<R(P)\\ V_0(P), & \rho\geq R(P)\end{cases} \tag{8}$$

where $R(P)$ is the wire radius. The variation of $R(P)$ is given by

$$R(P)=R_0(1-1.5082\times10^{-3}P) \tag{9}$$

$V_0(P)$ is the barrier height as a function of pressure and is given by [24]

$$V_0(P)=0.6\Delta E_g(x,P) \tag{10}$$

The Eigen functions of the Hamiltonian in Eq. (2) are

$$\psi_0(\rho,\phi,z)=N_0e^{im\phi}e^{ik_zz}U(\rho),\quad m=0,\pm1,\pm2,\ldots \tag{11}$$

where N_0 is normalization constant, k_z is the axial component of the electron's wavevector, $U(\rho)$ and $e^{im\phi}$ are the radial and angular parts of the electron wave function. $U(\rho)$ is given a linear combination of Bessel $J[n,\rho]$ function and appropriate Bessel $K[n,\rho]$ function. For the ground state

$$U(\rho)=\begin{cases}N\,\text{Bessel}J[0,r_{01}\rho], & 0\leq\rho\leq R(P)\\ N\dfrac{\text{Bessel}J[0,r_{01}R(P)]}{\text{Bessel}K[0,b_{01}R(P)]}\text{Bessel}K\left[0,b_{01}\rho\right], & \rho>R(P)\end{cases} \tag{12}$$

where N is normalization constant. Ground state electronic energies without Coulombic interaction $E(P)$ are given in terms of r_{01} and b_{01}. These values are obtained from the boundary conditions $(\psi_{inside}|_{\rho=R(P)}=\psi_{outside}|_{\rho=R(P)})$, $\left(\frac{d\psi_{inside}}{d\rho}\Big|_{\rho=R(P)}=\frac{d\psi_{outside}}{d\rho}\Big|_{\rho=R(P)}\right)$ and given by

$$r_{01}=\sqrt{\frac{2m^*(P)E(P)}{\hbar^2}-k^2}\quad\text{and}\quad b_{01}=\sqrt{\frac{2m^*(P)(V_0(P)-E(P))}{\hbar^2}+k^2} \tag{13}$$

when the impurity interaction is included, we use solution of Eq. (11) multiplied by a trial wave function chosen as $e^{-\lambda\sqrt{\rho^2+z^2}}$, where λ is variational parameter, that is to be determined by minimizing the expectation value of the Hamiltonian in the presence of the Coulombic interaction [25]. Therefore, the trial wave function for the system with the impurity is given by

$$\psi(\rho,z)=\begin{cases}N\,\text{Bessel}J[0,r_{01}\rho]e^{-\lambda\sqrt{\rho^2+z^2}}, & 0\leq\rho\leq R(P)\\ N\dfrac{\text{Bessel}J[0,r_{01}R(P)]}{\text{Bessel}K[0,b_{01}R(P)]}\text{Bessel}K\left[0,b_{01}\rho\right]e^{-\lambda\sqrt{\rho^2+z^2}}, & \rho>R(P)\end{cases} \tag{14}$$

Hydrogenic impurity binding energy E_b is defined as energy difference between energy of the system with and without Coulombic interaction. That is

$$E_b(R(P),P)=\langle H_0\rangle-\min_\lambda\langle H(R(P),P)\rangle \tag{15}$$

After some algebra parallel to no pressure case [26], hydrogenic impurity binding energy as a function of λ in terms of scaled parameters (scaled with Rydberg constant, for $P=0$ $R_B=(m^*e^4/2\varepsilon_0^2(\hbar^2))$ and Bohr radius $a_B=(\varepsilon_0\hbar^2/m^*e^2)$) is given as

$$\tilde{E}_b(R(P),P)=-(\lambda a_B)^2-4a_B\frac{[I_1+I_2]}{\partial/(\partial\lambda)[I_1+I_2]} \tag{16}$$

where I_1 and I_2 represent integrals that need to be calculated numerically and given below in dimensionless units with the following change of variable: $\rho=tR$

$$I_1=R^2(P)\int_0^1 tJ_0^2(r_{01}tR(P))K_0(2\lambda R(P)t)\,dt \tag{17}$$

$$I_2=R^2(P)\frac{J_0^2(r_{01}R(P))}{K_0^2(b_{01}R(P))}\int_1^\infty tK_0^2(b_{01}tR(P))K_0(2\lambda R(P)t)\,dt \tag{18}$$

In these integrals, J_0 and K_0 are the Bessel function of order zero [27]. Hence, Eq. (16) can be numerically solved for a specific λ value that minimizes it for any given P and $R(P)$ values.

Table 1
The pressure dependency of characteristic parameters of $Ga_{0.7}Al_{0.3}As$.

P (GPa)	$R(P)$ (Å)	$m^*(P)$ (A.U.)	$\varepsilon(P)$	$V_0(P)$ (meV)
0	103.72	0.067	13.13	227.88
5	102.68	0.099	12.69	216.18
10	101.64	0.146	12.25	204.48
15	100.60	0.216	11.81	192.78
20	100.50	0.319	11.37	181.08
25	99.77	0.47	10.93	169.38

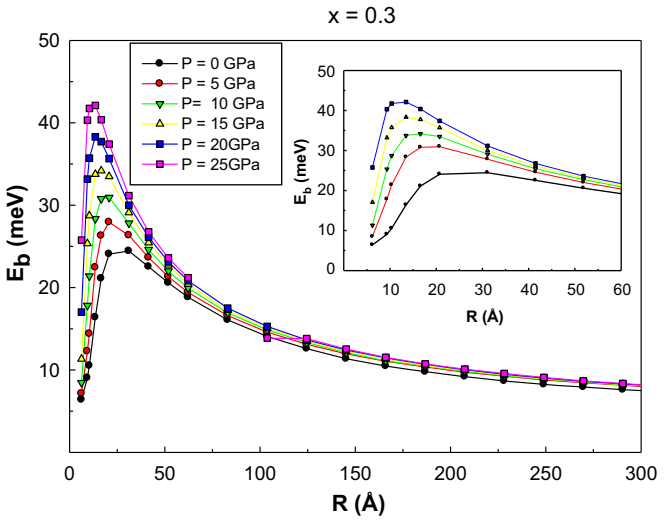

Fig. 1. Ground state binding energy E_b of hydrogenic impurity as a function of the wire radius for different values of external pressure.