IOP Conf. Series: Materials Science and Engineering **73** (2015) 012100 doi:10.1088/1757-899X/73/1/012100

Effect of Γ-X band mixing on the donor binding energy in a Quantum Wire

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Abstract. To invoke the technological applications of heterostructure semiconductors like Quantum Well (QW), Quantum Well Wire (QWW) and Quantum Dot (QD), it is important to understand the property of impurity energy which is responsible for the peculiar electronic & optical behavior of the Low Dimensional Semiconductor Systems (LDSS). Application of hydrostatic pressure P>35kbar drastically alters the band offsets leading to the crossover of Γ band of the well & X band of the barrier resulting in an indirect transition of the carrier and this effect has been studied experimentally and theoretically in a QW structure. In this paper, we have investigated the effect of Γ-X band mixing due to the application of hydrostatic pressure in a $GaAs/Al_xGa_{1-x}As$ QWW system. The results are presented and discussed for various widths of the wire.

1. Introduction

Confinement of hydrogenic impurity states in nanostructured systems and changes in the energy bands due to external perturbations lead to innovations in the field of band engineering and electronics. So far, a lot of theoretical and experimental investigations on hydrogenic impurity states in Low Dimensional Semiconducting Systems (LDSS) have been carried out worldwide by many researchers [1-3].The influence of position of donor impurity in quantum wire have been investigated theoretically for ground state and some excited states by A. Latge [4] et. al., and a comparative study between donor binding energy in cylindrical and rectangular quantum wire was made by Bryant [5]et. al., Brown and Spector [6] discuss confinement of carrier in Quantum wire with infinite and finite potential barriers. Navaneethakrishnan et. al., have investigated the effect of dielectric screening on the donor states [7] and on the diamagnetic susceptibility [8] of the donor. Tuning the band offsets is possible by applying external perturbations like electric [9] and magnetic field [10], laser field [11], pressure, etc.; Application of pressure on LDSS not only changes the dimensions of the system, but also alters the band gap through the mixing of Γ and X conduction bands in the well and in the barrier regions [12]. Experimental realization on Γ –X mixing in $GaAs/Al_xGa_{1-x}As$ coupled quantum wells under pressure was achieved by J.H.Burnett [13]. Recently the same effect has been investigated theoretically in single quantum well including the effect of non parabolicity of the conduction band by Nithiananthi [14] et.al.,

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In the Present work we investigate theoretically the effect of Γ-X on the ground state binding energy of a donor under hydrostatic pressure which is confined in a GaAs/$Al_xGa_{1-x}As$ Quantum wire by using variational method in the effective mass approximation, in view of exploring the technological applications in optics and electronics due to band tailoring.

2. Theory

The pressure dependent Hamiltonian of the donor electron in a GaAs-$Ga_{0.7}Al_{0.3}As$ quantum wire in atomic units is given by

$$\boldsymbol{H} = \frac{-\nabla^2}{2m^*_{w,b}(P)} - \frac{1}{\varepsilon_{w,b}(P)\boldsymbol{r}} + V_B(r,P) \quad (1)$$

where $m^*_{w,b}$ is pressure dependent effective mass of electron in well and barrier is given by[14]

$$m^*_W(P,T) = 1 \Big/ \left[1 + 7.51\left\{2/\Gamma_W(P,T) + \left[\Gamma_W(P,T) + 0.341\right]^{-1}\right\}\right] \quad (2)$$

$\Gamma_w(P,T)$ is the pressure dependent energy gap of GaAs at the Γ point and is given by[14]

$$\Gamma_w(P,T) = 1.519 + \alpha_w^\Gamma P - 5.405 \times 10^{-4}\, T^2 / (T + 204) \qquad (T = 4\ K) \quad (3)$$

where α_w^Γ is the pressure coefficient of GaAs at the Γ point

The barrier $Al_xGa_{1-x}As$ effective mass[15] $m^*_b(P,T) = m^*_w(P,T) + 0.083\,x$, x being Al composition.

The pressure dependent dielectric constant for GaAs and $Al_xGa_{1-x}As$ are given by

$$\varepsilon_w(P) = \varepsilon_w(0)\exp(\delta P) \quad (4)$$

where $\varepsilon_w(0) = \varepsilon_0(T_0)\exp[\gamma_0(T-T_0)]$ and

$$\varepsilon_b(P) = \varepsilon_w(P) - 3.12\,x \quad (5)$$

Pressure dependent potential energy of $Al_xGa_{1-x}As$ barrier is

$$V_B(r, P) = \begin{cases} 0 & |x|,|y| \le L(P)/2 \\ V_0(r, P) & |x|,|y| > L(P)/2 \end{cases} \quad (6)$$

$$V_0(r,P) = \begin{cases} \Gamma_b(P,T) - \Gamma_W(P,T) & P \le P_1 \\ X_b(P,T) - \Gamma_W(P,T) + S_{\Gamma X}(P) & P_1 < P < P_2 \end{cases} \quad (7)$$

The pressure dependent Γ - X band mixing strength coefficient

$$S_{\Gamma X}(P) = S_0\, x\, (P-P_1) / P \quad (8)$$

where S_0 (=250 meV) is the adjustable parameter. P_1 and P_2 are the critical crossover pressures between X_b - band and Γ_b - band and X_b - band and Γ_w - band respectively.

The variation of X_b band with pressure is $X_b(P) = X_b(0) + \alpha_b^X P$

α_b^X being the pressure coefficient for the barrier

Choosing the trial wave function of the donor impurity in its ground state as

$$\Psi_{1s} = N_{1s}\begin{cases} \cos \alpha x \cos \alpha y\, e^{-\alpha_{1s}\boldsymbol{r}} & |x|,|y| \le L(P)/2 \\ Be^{-\beta(x+y)} e^{-\alpha_{1s}\boldsymbol{r}} & |x|,|y| > L(P)/2 \end{cases} \quad (9)$$

$$\alpha = \sqrt{\frac{2m_W E(P)}{2}} \quad \text{and} \quad \beta = \sqrt{\frac{2m_b(P)[V_0(P) - E(P)]}{2}}$$

The variation of the width of the well as a function of the pressure[14] is given by

$$L(P) = L(0)[1-(S_{11}+2S_{12})P] \quad (10)$$

where S_{11} (=1.16 x 10^{-3} $Kbar^{-1}$) and S_{12} (= -3.7 x 10^{-4} $Kbar^{-1}$) are the elastic constants of GaAs and the pressure dependent subband energy is obtained by solving the transcendental equation

$$\tan\alpha\ L(P)/2 = \left[\frac{m_w^*(P,T)}{m_b^*(P,T)}\left(\frac{V_0(P)}{E(P)} - 1\right)\right]^{1/2} \tag{11}$$

The normalization constant B is obtained by applying the boundary conditions at $x = y = \pm L(P)/2$ on the wavefunction.

The pressure dependent binding energy is given by

$$E_B(P,T) = E(P,T) - \langle H(P,T)\rangle_{min} \tag{12}$$

3. Result and Discussion

The variation of the binding energy of the ground state donor with pressure in a quantum wire has been calculated and it is given in figure 1.

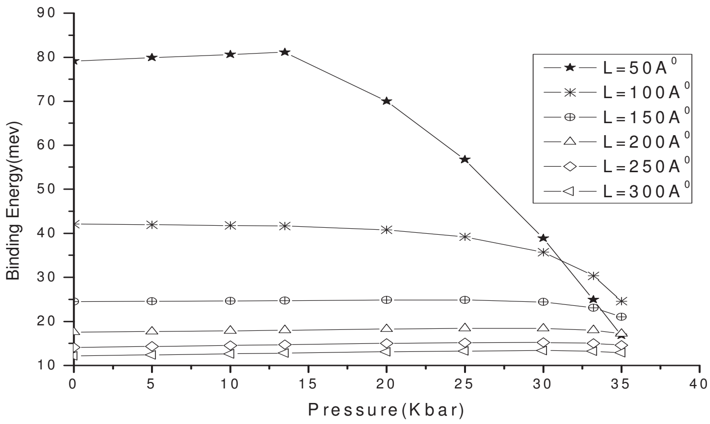

Figure 1:- Variation of binding energy as a function of pressure for various well widths.

From the figure, it is clear that up to $P \leq 13.5$ Kbar, binding energy of the donor increases with pressure due to the increase of effective mass and decrease of static dielectric constant. These factors decrease the kinetic energy and increase the potential energy of the donor respectively. And also, the potential barrier height remains constant in this region. Hence, the donor binding energy increases with pressure in this region for all sizes of the wire. After crossing the first critical pressure (P_1=13.5kbar), for smaller wire size, (L(P)=50Å), the donor impurity is found to be less bound with its host. This is due to the crossover of X band of barrier below the Γ band of barrier, which reduces the potential barrier height. When the size of the wire is increased, the rate of decrease of binding energy is reduced, which manifests the fact that the effect of Γ –X band mixing in the barrier is significant for smaller wires, even after pressure P_1. There is further decrease in the binding energy of the donor after second critical pressure (P_2=33.2kbar) due to the Γ –X band crossover in the well region also. Thus the system enters into an indirect band gap regime.

Figure 2 gives the behavior of binding energy with wire size for different pressures (P=0, P_1, P_2). The figure shows that the confinement of the donor impurity in Quantum wire is more for wires of smaller size for all pressure values. The characteristic behavior of a low dimensional wire is reflected in this figure with turnover in the value of binding energy, and shift in the peak value towards the lower width region.

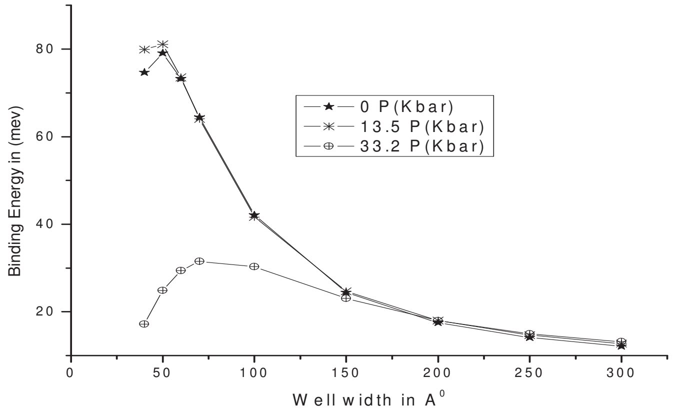

Figure 2:- Variation of binding energy as a function of well widths for various pressures.

To conclude, the effect of Γ –X band crossover is very significant in the lower width region even after P_1 which is seen from the drastic reduction in the binding energy for L(P)=50Å. The effect is very less in the higher well width region, (L (P) >200Å) and the localization of the donor is uniform which reflects the bulk behaviour. For wire sizes 50Å<L (P) <200Å, there is reduction in the donor binding only after P_2, which is similar to the behaviour observed in Quantum wells [14].

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