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Effects of spatially dependent effective mass and non-parabolicity on hydrogenic impurity binding energy in a near triangular quantum well

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Abstract - *Low dimensional semiconducting systems like quantum wells, wires and dots are extensively studied due to their applications in various fields. Near triangular quantum wells have attracted considerable attention of the researchers because of its applications such as speed circuits, optical devices etc. The effects of spatially dependent effective mass and nonparabolicity of conduction band on hydrogenic impurity binding energy in near triangular quantum well composed of GaAs/ $Ga_{1-x}Al_xAs$ have been investigated by variational method as a function of wellwidth and Al concentration. The spatially dependent effective mass (SDEM) affects the hydrogenic impurity to be less bound than that without the SDEM. Nonparabolicity of conduction band affects the hydrogenic impurity to be less bound than that without the non-parabolicity. The observed results are compared with those available in the literature.*

Key Words: Quantum well, Hydrogenic impurity, Binding energy, Spatially dependent effective mass, Non-parabolicity.

1.INTRODUCTION

The most significant nanostructures required to design nanoelectronic devices are Quantum Wells, Quantum Wires and Quantum Dots. In recent years, a great deal of interest has been shown in the properties of electron states in various quantum well structures. Experimental and theoretical researches have been made on the energies of electron states in a parabolic quantum well (PQW) with and without including the effect of spatially dependent effective mass (SDEM).

The binding energy of the ground state hydrogenic donor in Rectangular quantum well (RQW) has been calculated without [1] and with applied magnetic field [2]. The effect of a constant electric field on the energy position of the ground state exciton was studied in RQW [3]. The temperature dependence of the binding energy of shallow donors was reported in RQW [4]. The effect of non-parabolicity on hydrogenic donor binding energy in RQW was determined without and with an applied magnetic field [5]. The effect of magnetic field on exciton binding energy in Near triangular quantum well (NTQW) composed of GaAs-$Al_xGa_{1-x}As$ has been calculated as a function of wellwidth and Al concentration [6].

Qi et al [7] have calculated the effect of SDEM on hydrogenic impurity binding energy in a finite PQW as a function of wellwidth. Peter et al [8] have investigated the effects of both SDEM and DSF on hydrogenic donor binding energy in a quantum dot of GaAs/GaAlAs. Abarna et al [9] have theoretically studied the effects of dielectric screening function and image charges on hydrogenic donor binding energy in a surface quantum well made of vacuum/GaAs/$Ga_{1-x}Al_xAs$.

In this paper, the effect of SDEM on the hydrogenic impurity binding energy in a NTQW formed by GaAs-$Al_xGa_{1-x}As$ have been calculated and the results are compared with the available data.

2. THEORY

The Hamiltonian of hydrogenic impurity in a NTQW in the effective mass approximation can be written as [10]

$$H = -\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} - \frac{\partial^2}{\partial z^2} + V(z) - \frac{2}{r} \qquad (1)$$

We have considered the growth axis of quantum well structures to be the z axis. $r = \sqrt{\rho^2 + z^2}$, ρ is the distance in x-y plane.

The effective Rydberg R* is used as the unit of energy ($R^*=m^*e^4/2\hbar^2\epsilon_o^2$) and the effective Bohr radius a^* as the unit of length ($a^*= \hbar^2\epsilon_o/m^*e^2$), where $m^*$is the effective mass of the electron. The potential profile for electron in NTQW is

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given by [10], $$V(z) = \begin{cases} V_o \left|\frac{z}{L/2}\right|^{2/3} & |z| < L/2 \\ V_o & |z| > L/2 \end{cases}$$ (2)

where V_o is the barrier height, which depends on the composition x of Al. The trial wave function of the electron in NTQW is of the form [10],

$$\Psi = \begin{cases} Ne^{-\alpha^2 z^2} e^{-ar}; & -\frac{L}{2} \le z < L/2 \\ N_1 e^{-\beta z} e^{-ar}; & z > L/2 \\ N_1 e^{\beta z} e^{-ar}; & z < L/2 \end{cases} \quad (3)$$

Here α, β and a are the variational parameters. N is the normaliation constant. <H> was evaluated as a function of variational parameters using the Hamiltonian in equation (1) and trial wave function in (3).
The binding energy is given by

$$E_B = E_o - \langle H \rangle_{min} \quad (4)$$

where, E_o is the ground state energy of electron and $\langle H \rangle_{min}$ is the minimized value of $\langle H \rangle$ with respect to the variational parameters.
The expression for spatially dependent effective mass in given by [7],

$$m_1^* = 1 + 0.4018 \frac{z^2}{(L/2)^{2/3}} \quad (5)$$

Nonparabolicity of conduction band is given by [5],

$$m(E_e) = 0.0665 \left(1 + \frac{0.0436E_g + 0.236E_g^2 - 0.147E_g^2}{0.0665}\right) m_o \quad (6)$$

where E_o^* is the non-parabolicity parameter.

3. RESULTS AND DISCUSSION

For GaAs, we have m_e = 0.0665 m_o and ϵ_o = 13.2. The difference of total band gap between $Ga_{1-x}Al_xAs$ and GaAs is determined by [10],

$$\Delta E_g = 1.155x + 0.37x^2 \quad (6)$$

In figure 1, we have presented the variation of effective mass as a function of position of the donor for different wellwidths. It is observed that the effective mass increases when the value of z increases. For L=10 nm, the effective mass has higher values when compared with the other values of L= 20 nm and 30 nm.

In figure 2, we have displayed the variation of donor binding energy as a function of wellwidth with and without including the SDEM for x = 0.3. It can be seen from the figure that the binding energy of hydrogenic impurity increases as the wellwidth decreases up to 20 nm, due to the compression of wavefunction of donor in the well region. But for further reduction of the wellwidth, the binding energy starts to decrease and the reason is the spread out of the wave function into the barrier. When the effect of SDEM is included, the binding energy increases for strong confinement and it is insensitive to SDEM for weak confinement.

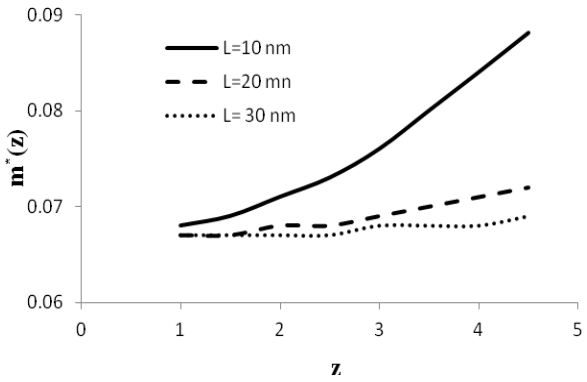

Fig-1: Variation of of $m^*(z)$ for various positions with different wellwidth

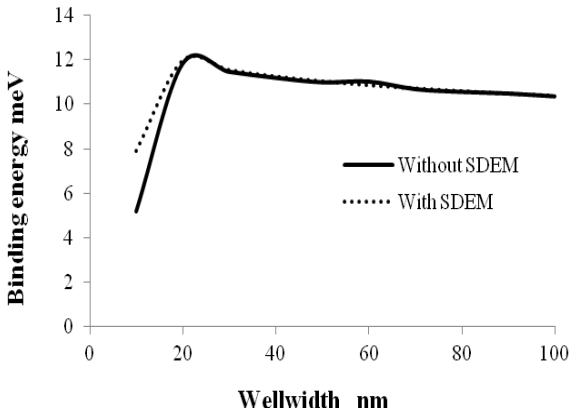

Fig-2: Variation of Binding energy as a function of wellwidth with and without SDEM .

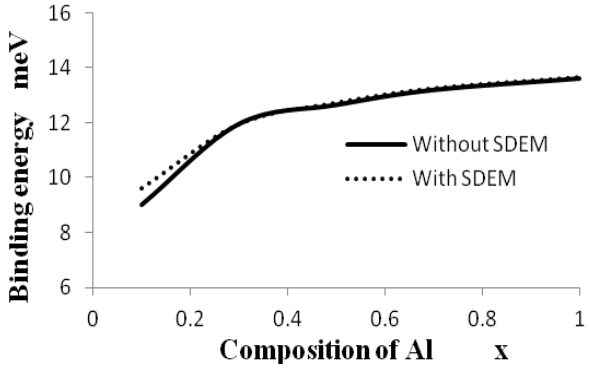

Fig-3: Variation of binding energy for various composition of x with and without SDEM for L = 20 nm

In figure 3, we have presented the variation of donor binding energy as a function of Al composition x with and without including the SDEM for L = 20 nm. It is observed that the binding energy E_B increases as composition of Al (x) increases for $x \leq 0.3$ due to the raise of the barrier height. For $x > 0.3$, the binding energy increases by a very less value. When the effect of SDEM is included, the binding energy shows an increase upto $x \leq 0.3$ beyond which, it is independent of x.

In figure 4, we have displayed the variation of donor binding energy as a function of wellwidth with and without including the SDEM for $x = 0.3$ including the effect of nonparabolicity. It is observed that the binding energy of donor with nonparabolicity is larger than that of without nonparabolicity.

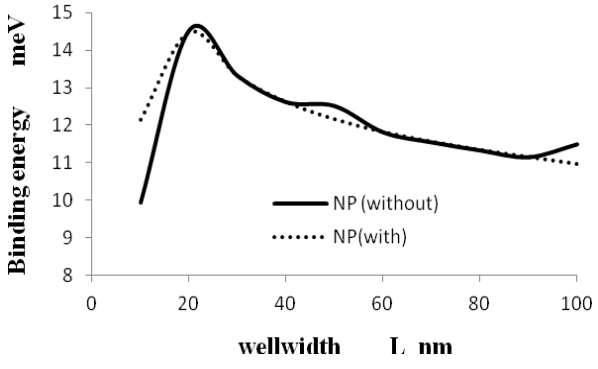

Fig-4: Variation of Binding energy as a function of wellwidth with and without SDEM by including the effect of nonparabolicity

In figure 5, we have presented the variation of donor binding energy as a function of Al composition x with and without including the SDEM for L = 20 nm by including the effect of nonparabolicity.

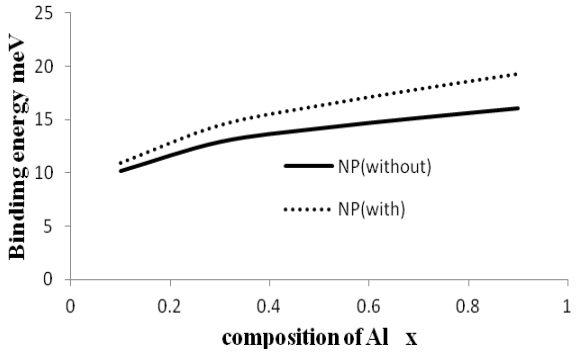

Fig-5: Variation of binding energy for various composition of x with and without SDEM for L = 20 nm including the effect of nonparabolicity

4. CONCLUSIONS

We have calculated the binding energy of donor impurity in NTQW composed of GaAs/$Ga_{1-x}Al_xAs$ as a function of wellwidth and Al composition including and excluding the SDEM. The results show that value of $m_1^*(z)$ increases as a function of position and binding energy of donor impurity increases when the SDEM and nonparabolicity are included.

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