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COMPOSITIONAL EFFECTS ON SHALLOW DONOR BINDING ENERGY OF A NANO DOT

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A theoretical study of a shallow donor binding energy in GaAs/$Ga_xIn_{1-x}Sb$ nano dot for different composition using a variational ansatz within the effective mass approximation was presented. The estimated donor binding energy as a function of dot radius (R) and composition shows that the binding energy increases as the size of the dot approaches from bulk to nano limit (1 Å – 10 Å) and binding energy increases abruptly for R < 20 Å due to quantum confinement effect. Increasing the concentration cause the further increment in the binding energy.

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1. Introduction

With the development of experimental techniques such as molecular-beam epitaxy, metal-organic chemical-vapor deposition, and electron-beam lithography combined with reverse-mesa etching, there has been much work devoted to the study of the states of hydrogenic impurities in lowdimensional semiconductor heterostructures such as quantum wells (QW's), quantum-well wires (QWW's), and quantum dots (QD's) [1-4]. They pay the way to fabricate many quantum well structures with dimensions comparable to the electronic de-Broglie wavelength. Due to their reduced dimensionality, these structures exhibit some physical properties such as optical and electrical transport characteristics that are more pronounced than those of bulk semiconductor constituents [5-6].

Theoretical studies for the binding energy of the ground state in GaAs QW's, [1] infinite QWW's, [7] and QD's [8] have shown that for an infinite confinement potential the binding energy increases monotonically as the finite dimension (length or radius) is reduced, whereas for finite confinement potential the binding energy increases up to a maximum and then begins to decrease. Studies for donor-doped QW's [1] and infinite QWW's [7] have shown that the binding energy present a maximum when the impurity is located at the center of the structure and decreases for positions close to the edges. It is anticipated that the fabrication of semiconductor quantum structures with zero dimensions will show exotic electronic behaviour such as the observation of discrete electronic states in GaAlAs/GaAs nanostructures due to the electronic confinement [9]. The impurity plays a fundamental role in some physical properties such as optical and transport phenomena at low temperature. The binding energy and the density of states of shallow impurities in cubic [10] and in spherical quantum dot [11] have been calculated as a function of dot size. The study of impurity states in semiconductor states is imperative as the addition of impurities can change the properties of any quantum device dramatically.

Using the variational method, Porras-Montenegro et al., [12] have studied a hydrogenic impurity in spherical QD systems with both infinite and finite barriers. The results reveal that, as the size of the QD decreases for an infinite barrier, the binding energy of the impurity increases monotonically, and for a finite barrier, the binding energy increases to their maxima and then sharply decreases. The effect of parabolic confinement on the binding energy of shallow hydrogenic impurities in a spherical quantum dot has been computed as a function of the dot dimension for different impurity positions and also as a function of the impurity position for different dot sizes for the infinite case [13] They show that the impurity binding energy increases with the reduction in the dot dimension. Also the binding energy is found to depend on the location of the impurity, and the same is the maximum for the on-centre impurity.

The most widely investigated quantum dot system is the GaAs/Ga1-xAlxAs system. But in our problem we have chosen to investigate GaAs/ In1-xGaxSb quantum dot. The quantum dot occurs in the GaAs region with InGaSb providing the barrier. If a donor is introduced in the GaAs region we have a simple hydrogenic donor, since GaAs is a direct gap material and the effective mass theory works well. However, if the size of the dot is small (~ 50 Å) the use of the effective mass theory is questionable. Effective mass theory is valid and usually employed in the studies of these properties.

In the present work, calculations of binding energies of the donor impurity in GaAs quantum dot with the barrier of GaInSb, placed at the centre are performed. Using the effective mass approximation, within a variational scheme, calculations are presented with constant effective mass (m*). The use of constant effective mass of 0.067 m_0 is justified for dot radius a*, where a* is an effective Bohr radius which is about ~ 100 Å . We have shown that the binding energy decreases as dot size increases. There is an increase of donor binding energy observed when the variation of concentration is included for all dot sizes. The adopted method and the results obtained from the said method are presented and discussed in the following section.

2. Theory

The Hamiltonian of a single hydrogenic shallow donor impurity, in a spherical GaAs quantum dot, in the effective mass approximation, is given by

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 - \frac{e^2}{\varepsilon_0 r} + V_D(r) \tag{1}$$

where ε_o is the static dielectric constant of GaAs

$$V_D(\bar{r}_j) = \frac{V_0 r^2}{R^2} \quad for \quad |r| \le R \quad while \quad V_D(\bar{r}_j) = V_0 \quad for \quad |r| > R$$

and V_0 is the barrier height of the parabolic dot given by $V_D(\bar{r}) = Q_c \Delta E_g(x)$. Q_c is the conduction band off-set parameter, which is taken to be 0.658 and the band gap difference between GaAs and $Ga_xIn_{1-x}Sb$ is given by [14]

$$\Delta E_g(x) = 0.235 + 1.653x + 0.413x^2 eV \tag{2}$$

The units of length and energy used throughout are the effective Bohr radius $R^* = \hbar^2 \varepsilon_o / m^* e^2$ and the effective Rydberg $R_y^* = m^* e^4 / 2\varepsilon_o^2 \hbar^2$ where ε_o is the dielectric constant and m* is the effective mass of electron in the conduction band minimum of GaAs with these values, R* = 103.7Å and R_y^* = 5.29meV.

By using these units, the Hamiltonian given in equation (1), becomes,

$$H = -\nabla^2 - \frac{2}{r} + V(r) \tag{3}$$

We have used a donor impurity in a quantum dot of GaAs. Since an exact solution of the Hamiltonian in equation (1) is not possible, a variational approach has been adopted.
The lowest state energies are obtained using the following wave function

$$\psi = \begin{cases} A\dfrac{\sin k_1 r}{r} & r \le R \\ B\exp(-k_2 r) & r > R \end{cases} \tag{4}$$

where, A and B are the normalization constants,
Here, $k_1 = (2m^* E/\hbar^2)^{1/2}$ and $k_2 = [2m^*(E-V)/\hbar^2]^{1/2}$. For a finite barrier case we choose the different concentration value and their respective barrier height is presented in the following table.

x	V(Ry*)	Eg(Ry*)
0.1	45.88905	0.40443
0.2	66.05083	0.58212
0.3	87.14983	0.76807
0.4	109.18606	0.96228
0.5	132.15952	1.16475
0.6	156.07021	1.37548

In a similar way as in the finite dot, inclusion of the impurity potential in the Hamiltonian forces to use of the variational approach. Then the trial wave function for the ground state with the impurity present is taken as

$$\psi = \begin{cases} N1\dfrac{\sin k_1 r}{r}\exp(-\beta_1 r), & r \le R \\ N2\exp(-k_2 r)\exp(-\beta_1 r), & r > R \end{cases} \tag{5}$$

where β_1 is the variational parameter and N_1, N_2 are normalization constants.

The ionization energy is given by

$$E_{ion} = E_{sub} - \langle H \rangle_{\min,} \tag{5}$$

where E_{sub} is the lowest sub band energy given by $E_{sub} = \dfrac{\hbar^2 k^2}{2m^*}$ with $k = \dfrac{\pi}{R}$

Thus the ionization energy is obtained, varying β_1 for different dot sizes with different concentration.

3. Results and discussion

Fig. 1 shows the sub band energy of the ground state with the different dot radius and different concentration values for a finite spherical GaAs quantum dot. In all the cases (different concentration values) the sub band energy decreases with increase of dot radius.

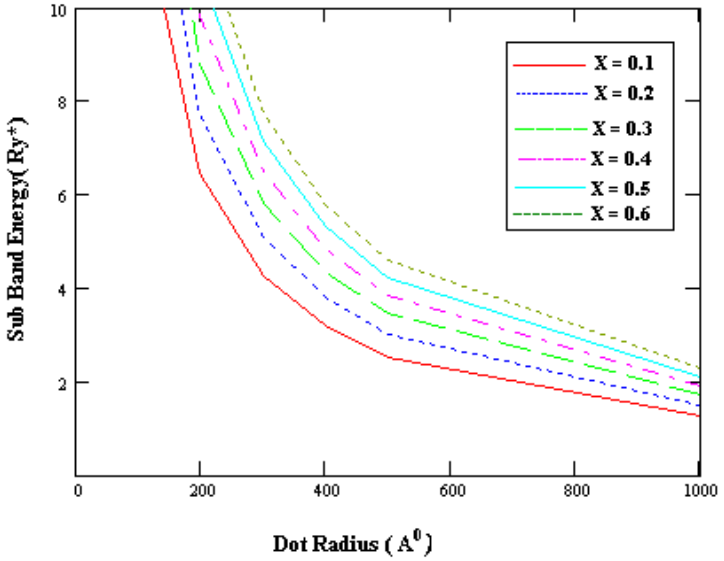

Fig. 1 Variation of Sub Band Energy with dot sizes for different concentrations

Fig. 2 represents the binding energy in a spherical GaAs/$Ga_{1-x}In_xSb$ quantum dot as a function of the dot radius for a hydrogenic donor. The binding energy increases as the dot radius decreases, reaches a maximum and then diminishes to a limiting value corresponding to a particular radius of the dot. It is observed that the binding energy goes to 1R* in the bulk limit for the larger radius. More over the binding energy of the dot vary with respect to concentrations. The binding energy is increased with the increase of concentrations. When the dot radius approaches the quantum limit (R < 100 Å), increase of binding energy is appreciable and reaches its maximum and suddenly it starts to diminish at (R < 20 Å) which shows in figure 3.

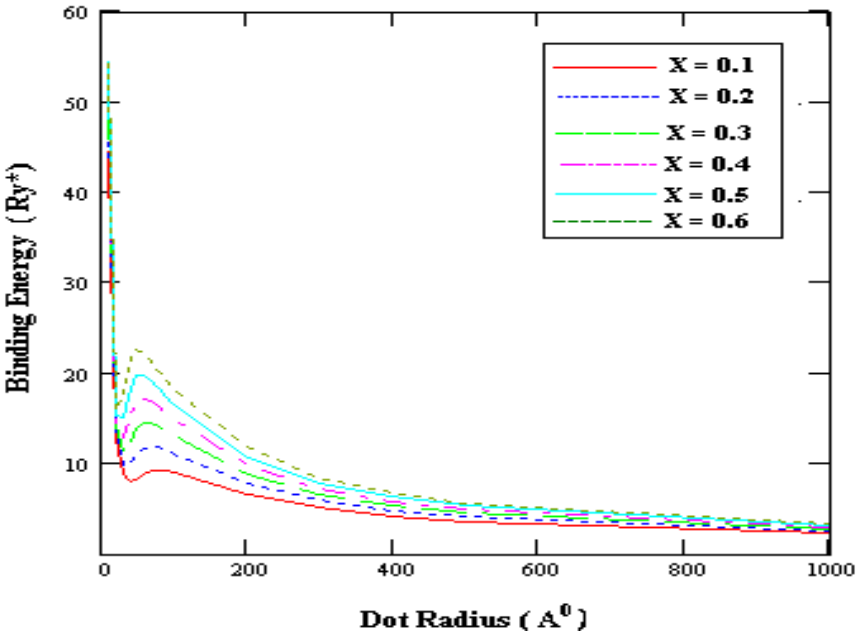

Fig. 2 Variation of Binding Energy with Dot sizes for different concentrations

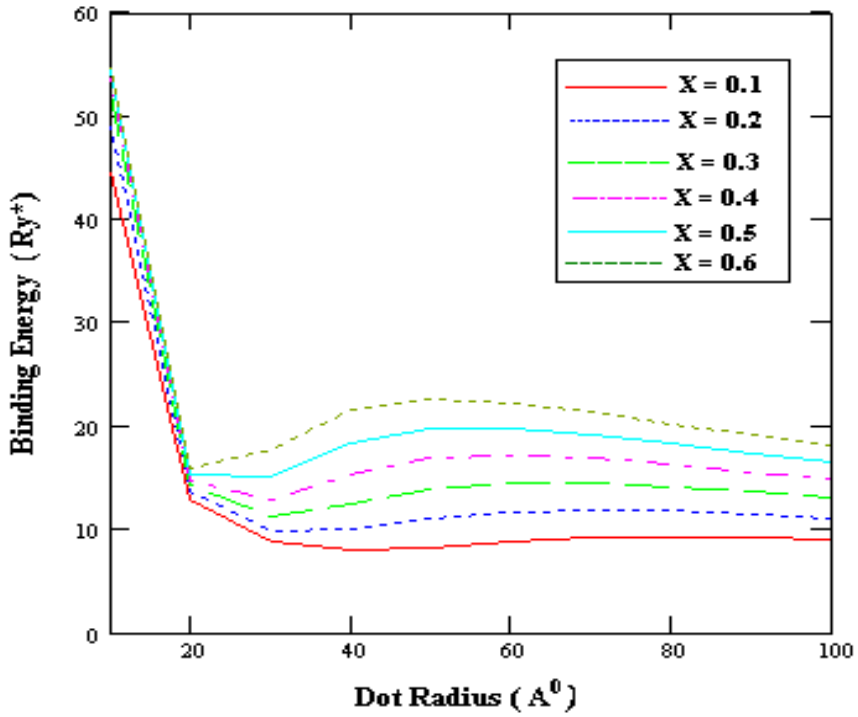

Fig. 3 Variation of Binding Energy with Dot sizes (Quantum limit) for different concentrations.

At a particular size of the dot such as R = 100 Å, the binding energy increased linearly with respect to concentrations and was shown in the figure 4.

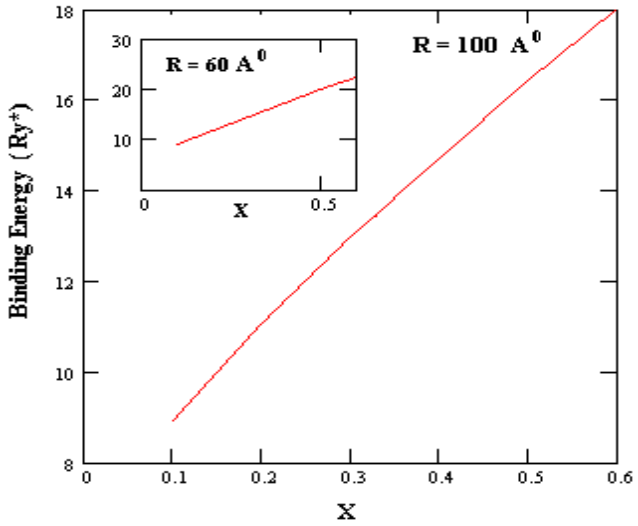

Fig. 4 Variation of Binding Energy with different concentrations for particular dot radius "R".

This clearly shows that concentrations play a significant role in the binding energy of quantum structures.

4. Conclusion

In conclusion, we can also tune the band gap of a quantum dot using concentrations of a barrier material as like as electric field, magnetic field and pressure. Tunabilty of band gap of this quantum dot plays significant role in luminescent and photovoltaic devices.

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