THE HYDROSTATIC PRESSURE EFFECT ON THE NORMALIZED INTRADONOR TRANSITION ENERGY IN A GAAS/$GA_{1-x}AL_xAS$ SPHERICAL QUANTUM DOT

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Abstract

In this study, the change of normalized intradonor transition energy depending on hydrostatic pressure is calculated using the variation method with the effective mass approach. Normalized intradonor transition energy is found using ground state (1s) and excited state (1p) impurity energies. It has been observed that the normalized inradonor transition energy increases with the quantum dot radius and hydrostatic pressure and decreases when the impurity moves from the center to the edge of the dot. Calculating the intradonor transition energy can make it possible to determine the position of the impurity in a spherical quantum dot. The results are in agreement with the studies found in the literature.

Keywords: normalized intradonor transition energy, hydrostatic pressure, variation method.

INTRODUCTION

Recently, many studies have been carried out on low-dimensional structures. These structures, especially quantum dots, attract significant attention in experimental and theoretical studies [1-7]. Effects such as hydrostatic pressure, temperature, electric field, magnetic field, and laser on quantum dots have been examined in detail [3,8,9]. There are studies calculating the effect of hydrostatic pressure on the binding energy of donor impurities in quantum dot (QW) structures [10-12]. Impurity plays a fundamental role in calculating physical properties, such as low-temperature optical and transport phenomena.

The exploration of subband energy level transitions in quantum dots has drawn significant interest, with researchers utilizing various solution methods to study their behaviour under different conditions such as hydrostatic pressure, temperature, laser, and magnetic field [13-17]. Calculating the intradonor transition energy, the difference in energy between the donor's ground state and its final state is crucial for understanding the optical properties of low-dimensional systems. In addition, studies are calculating the change in normalized intradonor transition energy depending on dot radius, temperature, and aluminium concentration in the spherical quantum dot [7,18]. Most weak features are not detectable in transition energy but can be observed by calculating normalized intradonor transition energy.

The study calculates the normalized intradonor transition energies between 1s and 1p states in a spherical quantum dot. It uses a variational approach within the effective mass approximation to determine the effects of dot radius, hydrostatic pressure, and impurity position on the calculation. For the first time, the study has determined the impact of hydrostatic pressure on normalized intradonor transition energy.

THEORY

Utilizing spherical coordinates and the effective mass approximation, derive the Hamiltonian for a single electron system containing a hydrogenic impurity inside a quantum dot given by [19]

$$H = -\frac{\hbar^2}{2m^*(P,T)}\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right) - \frac{A\,e^2}{4\pi\varepsilon_0\varepsilon(P,T)|r-r_i|} + \frac{B\,\hbar^2}{2m^*(P,T)}\frac{(l(l+1)}{r^2} + V(r,P,T) \quad (1)$$

The A and B are arbitrary constants. In this notation, the presence or absence of an impurity is denoted by 1 or 0. The B value is also defined using 0 or 1 to indicate the ground or excited states. Where P, T, $m^*(P,T)$, $V(r,P,T)$, $\varepsilon(P,T)$, and r_i are hydrostatic pressure, temperature, electronic effective mass, and confining potential, static dielectric constant and impurity position, respectively. In the calculations, the temperature is taken as constant T=4 K. For GaAs m^*(P,T) and ε(P,T) are defined as [20],

$$m^*(P,T) = \frac{m_o}{1+7.51\left[\frac{2}{E_g^{\Gamma}(P,T)}+\frac{1}{E_g^{\Gamma}(P,T)+0.341}\right]} \quad (2)$$

and

$$\varepsilon(P,T) = \begin{cases} 12.74\ exp\left[-1.73x10^{-3}\ P\right] exp\left[9.4x10^{-5}\ (T-75.6\ K)\right] & for\ T \le 200\ K \\ 13.18\ exp\left[-1.73x10^{-3}\ P\right] exp\left[20.4x10^{-5}\ (T-300\ K)\right] & for\ T \ge 200\ K\ . \end{cases} \quad (3)$$

Here, m_0 is the free electron mass. $E_g^{\Gamma}(P,T)$ is the energy band gap change depending on the hydrostatic pressure and temperature for the GaAs structure at the Γ point, and can be expressed as [10]

$$E_g^{\Gamma}(P,T) = 1.519 - \left[\frac{5.405x10^{-4}T^2}{T+204\ K}\right] + (1.26\times10^{-2})P - (3.77\times10^{-4})P^2\ . \quad (4)$$

In eq.1, V(r, P, T) is the confining potential and is defined as [21],

$$V(r,P,T) = \begin{cases} V_0(P,T) & ,\quad r \ge R(P) \\ 0 & ,\quad r < R(P) \end{cases} , \quad (5)$$

where $V_0(P,T) = Q_c\,\Delta E_g^{\Gamma}(x,P,T)$ and Q_c = 0.658. $\Delta E_g^{\Gamma}(x,P,T)$ is the total energy band gap difference between GaAs and $Ga_{1-x}Al_xAs$ barrier medium, and is given by [10, 20]

$$\Delta E_g^{\Gamma}(x,P,T) = \Delta E_g^{\Gamma}(x) + P\,D(x) + T\,G(x) , \quad (6)$$

Where, $\Delta E_g^{\Gamma}(x) = 1.155\,x + 0.37\,x^2\ in\ eV$, $D(x)$ and $G(x)$ are the pressure coefficients of the band gap, which are defined as

$$D(x) = -1.3\times10^{-3}\,x \quad in\ eV/kbar$$

and

$$G(x) = -1.15\times10^{-4}\,x \quad in\ eV/K\ .$$

The R(P) is a variation of the dot radius with pressure and is expressed as [22]

$$R(P) = R_0\ [\ 1-(1.16\times10^{-3}\ kbar^{-1} + 2\ (-3.7\times10^{-4}\ kbar^{-1}))\,P\ ] , \quad (7)$$

where, R_0 is the dot radius without hydrostatic pressure.

In the presence of impurity, the wave functions for the ground state (1s) and excited state (1p) of the spherical quantum dot system can be expressed as [7,18,23]

$$\psi_{1s}^{imp}(r,r_i)=\begin{cases}\left(N_{1si}^{sub}\,sin(k_{1si}r)/r\ \right)\exp\left(-\lambda_{1s}\sqrt{r^2+r_i^2-2rr_i\cos\theta}\right), & r\le R\\ \left(N_{1s0}^{sub}\exp\left(-(k_{1si}r)\right)/r\right)\exp\left(-\lambda_{1s}\sqrt{r^2+r_i^2-2rr_i\cos\theta}\right), & r\ge R\end{cases} \quad (8)$$

and

$$\psi_{1p}^{imp}(r,r_i)=$$
$$\begin{cases}N_{1pi}^{sub}\left(\frac{sin(k_{1pi}r)}{(k_{1pi}r)^2}-\frac{cos(k_{1pi}r)}{(k_{1pi}r)}\right)\mathrm{r}\cos(\theta)\exp\left(-\lambda_{1p}\sqrt{r^2+r_i^2-2rr_i\cos\theta}\right), & r\le R\\ N_{1p0}^{sub}\left(\frac{1}{(k_{1p0}r)}+\frac{1}{(k_{1p0}r)^2}\right)\exp\left(-k_{1po}r\right)\mathrm{r}\cos(\theta)\exp\left(-\lambda_{1p}\sqrt{r^2+r_i^2-2rr_i\cos\theta}\right), & r\ge R\end{cases} \quad (9)$$

where, λ_{1s} and λ_{1p} are variational parameters, N_{1s0}^{sub}, N_{1si}^{sub}, N_{1p0}^{sub} ,and N_{1pi}^{sub} refer to normalization coefficients, and

$$k_{1si}=\sqrt{2m^*(P,T)E_{1s}^{sub}/\hbar^2}$$
$$k_{1so}=\sqrt{2m^*(P,T)(V(r,P,T)-E_{1s}^{sub})/\hbar^2}$$
$$k_{1pi}=\sqrt{2m^*(P,T)E_{1p}^{sub}/\hbar^2}$$
$$k_{1po}=\sqrt{2m^*(P,T)\left(V(r,P,T)-E_{1p}^{sub}\right)/\hbar^2}. \quad (10)$$

The corresponding energy values, $E_{1s}^{sub}$and E_{1p}^{sub}, are obtained by the solutions of transcendental equations [7,22].

The energies are found by the variation method for the 1s and 1p impurity states, respectively. [18].

$$E_{1s}^{imp}=min_{\lambda_{1s}}\langle\psi_{1s}^{imp}|H^{A=1,B=0}|\psi_{1s}^{imp}\rangle/\langle\psi_{1s}^{imp}|\psi_{1s}^{imp}\rangle \quad (11)$$

and

$$E_{1p}^{imp}=min_{\lambda_{1p}}\langle\psi_{1p}^{imp}|H^{A=1,B=1}|\psi_{1p}^{imp}\rangle/\langle\psi_{1p}^{imp}|\psi_{1p}^{imp}\rangle. \quad (12)$$

Using 1s and 1p impurity energies, the normalized intradonor transition energy($NE_{imp1s1p}^{tran}$) is described as given by[7,18]

$$NE_{imp1s1p}^{Trans}=\left[E_{1p}^{imp}-E_{1s}^{imp}\right]/E_{1s}^{imp} \quad (13)$$

EXPOSITION

In this section, the $NE_{imp1s1p}^{tran}$ is calculated using the variation method under effective mass approximation as a function of hydrostatic pressure, SQD radius, and impurity location. In calculations, the aluminium (Al) concentration is used as constant x=0.3. The $NE_{imp1s1p}^{tran}$ results obtained for P=0 kbar agree with the studies in the literature [18]. The results for the variation of $NE_{imp1s1p}^{tran}$ depending on hydrostatic pressure, SQD radius, and impurity position are presented in Figures 1-3.

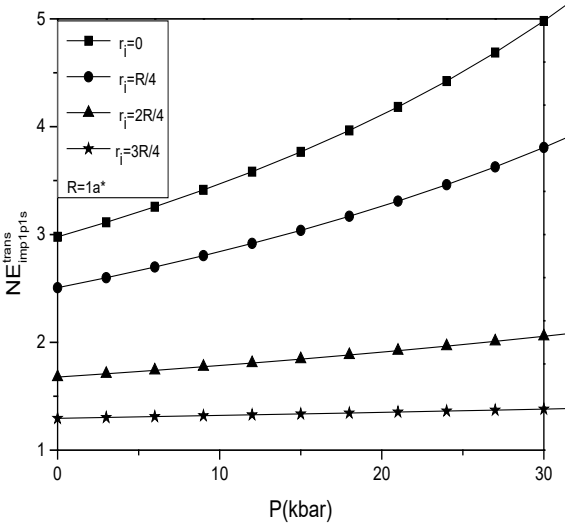

Fig. 1. *Change of $NE_{imp1s1p}^{tran}$ depending on hydrostatic pressure.*

In Figure 1, the change of the $NE^{tran}_{imp1s1p}$ depending on the hydrostatic pressure, is calculated for the R = 1a* radius of the spherical quantum dot and four different impurity positions. While the $NE^{tran}_{imp1s1p}$ is more affected by hydrostatic pressure when the impurity is close to the centre of the quantum dot, the effect of hydrostatic pressure is less when the impurity moves toward the edge. Thus, this graph, the change of $NE^{tran}_{imp1s1p}$ depending on hydrostatic pressure, can give us an idea about the location of the impurity within the quantum dot.

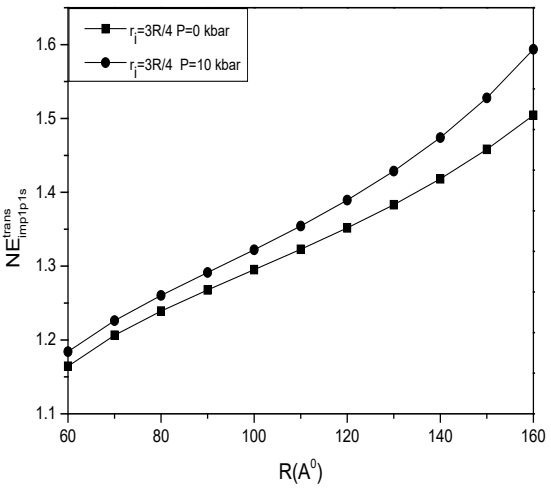

Fig. 2. *Variation of the $NE^{tran}_{imp1s1p}$ energy according to quantum dot radius.*

In Figure 2, the $NE^{tran}_{imp1s1p}$ variation depending on the quantum dot radius is investigated for the position r_i=3R/4 of the impurity and hydrostatic pressure P=0 and 10kbar. It is observed that the $NE^{tran}_{imp1s1p}$ increases with increasing quantum dot radius. In addition, at the position of the impurity r_i=3R/4, the pressure effect on the $NE^{tran}_{imp1s1p}$ is less pronounced at narrow quantum dots and more pronounced at wide quantum dots. Furthermore, we can get an idea of the radius of the quantum dot by looking at the difference between the $NE^{tran}_{imp1s1p}$ values for the pressure values P=0 and P=10 kbar.

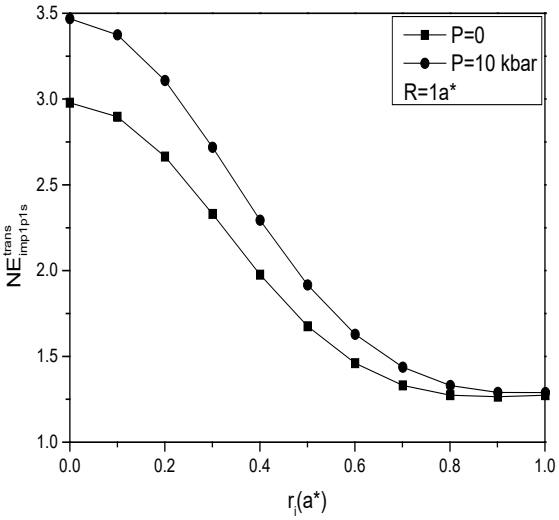

Fig. 3. *The $NE^{tran}_{imp1s1p}$ as a function of the impurity position.*

The change of the $NE^{tran}_{imp1s1p}$ depending on the impurity position is examined for R=1a* quantum dot width and hydrostatic pressure P=0, 10 kbar values in Figure 3. It has been observed that the $NE^{tran}_{imp1s1p}$ decreases when the impurity moves from the center to the edge of the quantum dot. In addition, it can be seen that when the impurity position is larger than r_i=3R/4, the $NE^{tran}_{imp1s1p}$ change remains almost constant. Moreover, the results found for the r_i=3R/4 position of the impurity are in agreement with the results found for the change of $NE^{tran}_{imp1s1p}$ with hydrostatic pressure in Figure 1.

CONCLUSION

In this study, the change of the $NE^{tran}_{imp1s1p}$ depending on the hydrostatic pressure, the quantum dot's radius, and the impurity's position is examined. As the impurity position approaches the edge of the quantum dot, the $NE^{tran}_{imp1s1p}$ remains almost constant. Moreover, hydrostatic pressure's effect on the $NE^{tran}_{imp1s1p}$ is more pronounced when the impurity is close to the quantum dot's center. At the same time, it becomes weaker when the impurity is close to the edge of the quantum dot. In addition, in narrow quantum dot radii,

the effect of hydrostatic pressure on the $NE_{imp1s1p}^{tran}$ is weaker.

In summary, calculating the change of the $NE_{imp1s1p}^{tran}$ depending on the hydrostatic pressure and the radius of the quantum dot can give us information about the position of the impurity.

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