

Potential Barrier Dependence of the Ground-state Recombination Energy in (In,Ga)N-GaN Spherical QD

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Within the framework of effective-mass approximation and finite parabolic potential confinement barrier we calculated the electron (hole) energy, average relative distance between carriers and uncorrelated ground-state ($1S_e - 1S_h$) electron-hole recombination energy in (In,Ga)N (well)-GaN (shell) spherical quantum dot nanoparticles. Furthermore, we investigated the potential barrier (Indium composition) and structure's radius effects. These results show that the recombination energy decreases according to the quantum dot radius for all indium composition. A critical value of spherical radius is obtained constituting the turning point limiting two potential barrier behaviors.

1. Introduction

In the past few decades, low-dimensional semiconductor systems (LDS) such as quantum well (QW), quantum well wire (QWW), quantum dot (QD), and quantum ring (QR) have attracted much interest due to their importance in physics, electronic and optical applications. The presence of impurities is one of the main problems in LDS since the electrical, optical and mechanical properties of the constituent semiconductor materials can be altered by these defects. A considerable amount of work has been devoted to the investigation of external perturbations on impurities-related physical properties in LDS [1-14].

The nanoparticles QD provide a flexibility to tailor electron and hole characteristics and then e-h optical recombination by changing the thickness of the well, which amounts to a three-dimensional example of properties engineering. This structure gives rise to a significant redistribution of carriers. Within the framework of the effective-mass approximation, Mews et al. [15] have investigated $1S_e - 1S_h$ recombination energy in HgS nanoparticles in which the coulomb interaction is not taken into account. Schooss et al. [16] investigated both theoretically and experimentally the coulomb interaction effect on $1S_e - 1S_h$ transition energy considering the finite barrier at the nanoparticle boundary. Many others materials,

such CdS [17,18], InAs [19,20], HgSe [21], ZnS [22], and InP [23] are reported. Additionally, the excited states electron-hole transition under the magnetic field in (Al,Ga)As is reported [24].

The most interesting novel features of QD nanoparticles is the inter-band recombination between electron and hole states localized in its internal well. This recombination gives rise to a new band gap observed experimentally, referred to as $1S_e - 1S_h$ recombination [15,16,25,26]. So far, for a QD layer with a narrow well layer less than three monolayers in thickness, all of the reported experimental results have concentrated on $1S_e - 1S_h$ recombination [15,16]. Thus, in the present paper, we have focused our study on electron and hole ground-states ($1S$) recombination energy under finite parabolic potential.

2. Theoretical Framework

We consider $\text{In}_x\text{Ga}_{1-x}\text{N}$ spherical quantum dot (SQD) of radius R immersed in GaN matrix ($r > R$). Generally, the confinement potential proposed for such a structure is of rectangular form. However, taking account of the mixing of components at the well and shell interface region, and the presence of the impurities especially in the growth period, it is suitable for this particular problem, to adopt the finite parabolic potential barrier given below as Eqn. (1).

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$$V^i = \begin{cases} \frac{Q^i \Delta E_g(x)}{R^2} r^2 & r \leq R \\ Q^i \Delta E_g(x) & \text{elsewhere} \end{cases} \quad i \equiv e, h \quad (1)$$

Where, Q^i (0.7, 0.3) denotes the conductor band offset of the conduction band and the valence band, respectively. The difference between GaN band-gap and $\text{In}_x\text{Ga}_{1-x}\text{N}$ band-gaps is

$$\Delta E_g(x) = E_g^{\text{GaN}} - E_g^{\text{In}_x\text{Ga}_{1-x}\text{N}}(x) \quad (2)$$

Where, $\text{In}_x\text{Ga}_{1-x}\text{N}$ band-gap is given as

$$E_g^{\text{In}_x\text{Ga}_{1-x}\text{N}}(x) = x E_g^{\text{InN}} + (1-x) E_g^{\text{GaN}} - 3.8x(1-x) \text{ (eV)} \quad (3)$$

It is well known that for spherical symmetric potential, the separation of radial and angular coordinates leads to a wave-function describing the electron states confined in SQD nanoparticle given as

$$\Psi_{nlm}(\vec{r}) = R_{nl}(r) Y_{lm}(\theta, \varphi) \quad (4)$$

Where, $Y_{lm}(\theta, \varphi)$ is the spherical harmonics and $R_{nl}(r)$ is the radial wave-function.

In the absence of hydrogenic impurity, the electron (hole) effective-mass Hamiltonian in such a structure can be given as

$$H_i = -\frac{\hbar^2}{2} \nabla \left(\frac{1}{m_i^*} \right) \nabla + V^i \quad (5)$$

Here, ∇ is the nabla operator, which is used since the mass will be treated as a radial-dependent variable and V^i is the potential barrier as mentioned above.

$$m_i^* = \begin{cases} x m_{i,\text{InN}}^* + (1-x) m_{i,\text{GaN}}^* & r \leq R \\ m_{i,\text{InN}}^* & \text{elsewhere} \end{cases} \quad (6)$$

The stationary Schrödinger equation for the radial wave function has the following form given by Eqn. (7).

$$\frac{d^2 R_i(r)}{dr^2} + \frac{2}{r} \frac{dR_i(r)}{dr} + \left[\frac{2m_i^*}{\hbar^2 (E^i - V^i(r))} - \frac{l(l+1)}{r^2} \right] R_i(r) = 0 \quad (7)$$

According to [27], and taking into account the fact that the desired solution behavior for $r \rightarrow 0$ and $r \rightarrow \infty$, the radial wave-function is given as follows

$$R^{n,l}(r) = \left(\frac{2}{r_{0,i}^2} \right)^{\frac{l}{2}} r^l F_l \left(-n, l + \frac{3}{2}, \frac{2r^2}{r_{0,i}^2} \right) \exp \left(-\frac{r^2}{r_{0,i}^2} \right) \quad (8)$$

Where, $F_l(r)$ is the confluent hyper-geometric-function defined for a positive integer n while r_0 is defined as

$$r_{0,i} = \frac{\sqrt{2\hbar R}}{(2m_i^* Q^i \Delta E_g)^{1/4}} \quad (9)$$

An infinite set of equidistant values of electron (hole) energy levels is obtained ($n = 0, 1, 2, \dots$), which is given as

$$E_n^i = \frac{\hbar^2}{m_i^* r_{0,i}^2} \left[2n + l + \frac{3}{2} \right] \quad (10)$$

Since the electron (hole) confinement energy is calculated relative to the conduction (valence) band, the uncorrelated ground-state electron-hole is obtained as the sum of the confinement energies of electron, hole and bulk band-gap of the composite material. It is given as

$$E_0^{\text{rec}} = E_0^e + E_0^h + E_g^{\text{(In,Ga)N}}(x) \quad (11)$$

The ground-state e-h wave-function in SQDQW nanoparticle is given as

$$\psi(r_e, r_h) = \exp(-\lambda |\vec{r}_e - \vec{r}_h|) R_e(r_e) R_h(r_h) \quad (12)$$

Where, λ is the variational parameter, whereas $R_e(r_e)$ and $R_h(r_h)$ are the radial eigen functions of the electron and the hole, respectively. The term $\vec{r}_e(\vec{r}_h)$ is the position vector of electron (hole) with the origin at the center of the SQDQW nanoparticle

while $r_{eh} = |\vec{r}_e - \vec{r}_h|$ is the relative distance between the electron and the hole.

For uncorrelated carriers ($\lambda = 0$), Eqn. (12) has the advantage of having a simple form. The average relative distance r_{eh} between the electron and hole can be defined as

$$\overline{r_{eh}} = \frac{\langle \psi(r_e, r_h) | r_{eh} | \psi(r_e, r_h) \rangle}{\langle \psi(r_e, r_h) | \psi(r_e, r_h) \rangle} \quad (13)$$

3. Results and Discussion

To get a good picture of e-h recombination energy in (In,Ga)N SQD as a function of the potential barrier effect (indium composition), we have primarily investigated the structural dimension effect on the electron (hole) energy level. As we have mentioned in the introduction, in commonly used QD nanoparticles with smaller radius, the 1S-state is the main confined state in the well. Fig. 1 shows the ground-state electron (hole) energy level as a function of $\text{In}_{0.2}\text{Ga}_{0.8}\text{N}$ QD's radius. As expected, the particle energy decreases when QD's radius increases for finally to tend to the corresponding $\text{In}_{0.2}\text{Ga}_{0.8}\text{N}$ bulk material. For a fixed QD's radius, the confinement effect is more sensitive by the electron than by the hole. This effect is more significant in smaller QD for both particles.

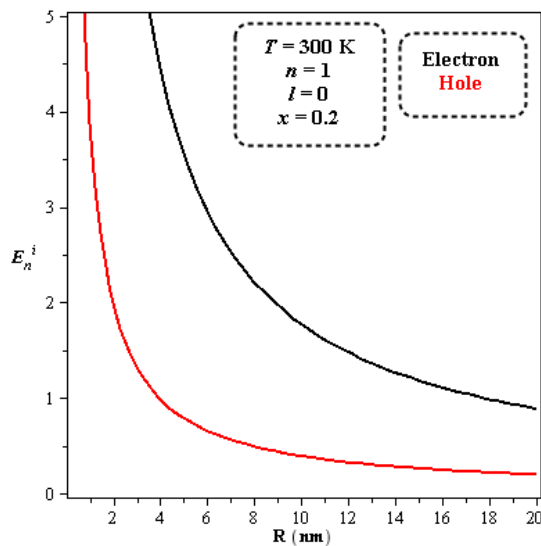


Fig.1: Ground-state electron (hole) energy level as a function of $\text{In}_{0.2}\text{Ga}_{0.8}\text{N}$ QD radius at room temperature.

The result of our calculation of the uncorrelated e-h recombination energy in (In,Ga)N-GaN SQD versus the QD's radius for three potential barriers are depicted in Fig. 2. It appears that the recombination energy decreases versus the QD radius for all indium fractions. This result confirms those obtained by Schooss et al. [16], who investigated both theoretically and experimentally the e-h correlation effect on $1S_e - 1S_h$ inter-band transition energy in CdS/HgS/CdS spherical layers under finite barrier. The main feature of these results is the fact that two behaviors are obtained, i.e., a critical value of the system radius is obtained that separates two different behaviors. For a given QD's radius, the e-h recombination energy increases according to the potential barrier (Indium fraction) for $R \leq R_c$ while it decreases as a function of In concentration in the composite material for $R \geq R_c$. This critical value is known as the turning point (TP). These results are in good agreement with those we have obtained in our previous work concerning GaN |(In,Ga)N| GaN spherical quantum dot-quantum well SQDQW [28]. We have shown that the critical radius (R_c) depends strongly on its inner radius, i.e., the more core radius increases, the more critical radius decreases.

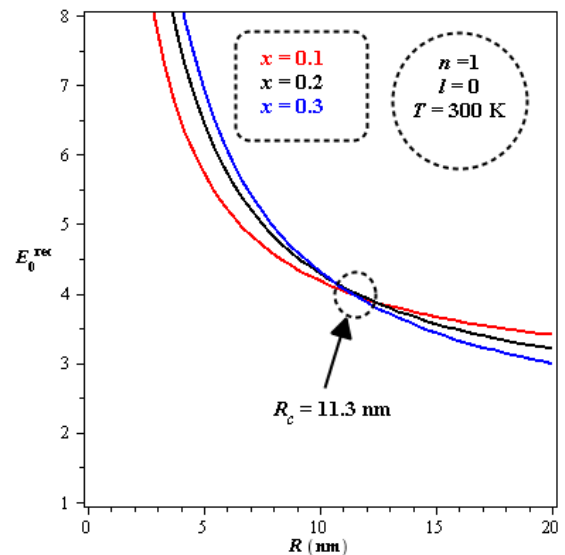


Fig.2: The ground-state e-h recombination energy versus the (In,Ga)N QD's radius for three potential barriers at room temperature.

In order to understand the results shown in Fig. 2, we further plot the average relative distance

between the electron and the hole in Fig. 3, which is directly related to recombination energy. Fig. 3 indicates that $\overline{r_{eh}}$ increases as a function of the QD radius for all indium concentrations. The principle feature of this figure is the similar behavior as that of e-h recombination energy, i.e., a critical value of the QD radius is obtained, which confirm the results presented in Fig. 2. Then, the change of inter-band recombination energy via the indium composition can be attributed to the average relative distance between electron and hole.

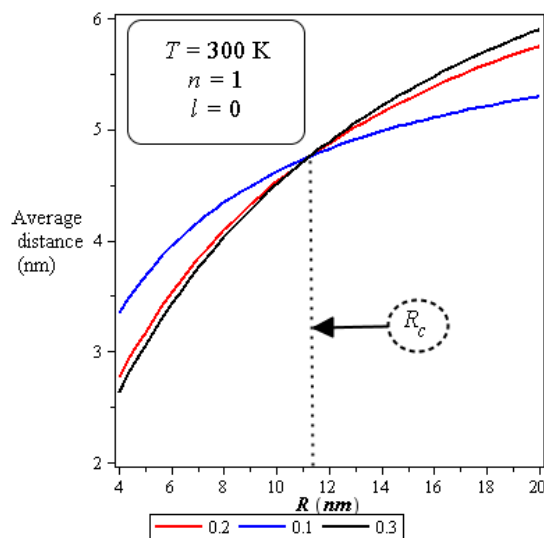


Fig.3: The average relative distance between the electron and the hole as a function of the SQD radius at room temperature for three potential barriers values.

Generally our numerical results are in good agreement with those reported in the literature. To the best of our knowledge, the turning behavior due to the potential barrier is not reported in the works cited above but this behavior is reported for SQD system based on GaAs material especially for external perturbations such as electric and magnetic fields. On the one hand, such turning behavior concerning excited states energy and binding energy under electric and magnetic fields as a function of SQD is obtained [24,29]. For GaAs material, it has been found that the impurity energy changes from negative to positive when the dot radius is smaller than $1.67a^*$ ($4.92a^*$) for 2S (2P) state. It is also obtained for each dot radius. There is a critical electric (magnetic) field strength for which the excited state energies change from positive to negative. The TP value is obtained for

electric field at 62.5KV.cm^{-1} (1.52KV.cm^{-1}) for SQD radius equals to $1.67a^*$ ($4.92a^*$) while it is obtained for magnetic field at $\gamma_0 = 0.06$ for $1.65a^*$ (2S state) and $\gamma_0 = 0.78$ for $4.92a^*$ (2P state). According to our recent paper concerning the lowest excited state binding energy in InGaN/GaN SQD, a critical value of the radius and the electric field is shown [30]. It is found that the energy level changes from positive to negative value as the electric field increases. The more the QD radius increases, the more the critical value of electric field decreases, i.e., it is equal respectively to $27.5F^*$ ($12.5F^*$) for the SQD radius is equal $3.2a^*$ ($5.2a^*$) (F^* is the effective electric field). Additionally, it is important to mention that the existence of the TP is also reported by Dane et al. [31]. The calculated value of TP is $1.852a^*$ for 1S state. Incidentally, for GaN/InGaN/GaN spherical quantum dot-quantum well (SQD-QW), the same behavior is obtained [32]. For a critical value of the outer shell and the inner core ratio, the inter-band transition in InGaN well changes its behaviors versus the indium concentration.

From the above discussion, it appears that the TP of optical and electrical properties under external perturbations is a characteristic of different semiconductor materials. Finally, we can speculate that the turning behavior concerning the recombination energy can be explained by the average relative distance between the carriers versus the indium fraction in the ternary alloy.

4. Conclusion

Electron eigenvalue, average relative e-h distance and uncorrelated e-h recombination energy in InGaN/GaN SQD nanoparticles are computed at room temperature. The QD's dimension and the Indium concentration effects are investigated within the framework of the single band effective-mass approximation and finite parabolic potential confinement barrier. The results we have obtained show that: (i) the electron (hole) eigenvalue decreases versus the system radius; (ii) the average relative distance increases according the QD radius for all indium fraction; (iii) the e-h recombination energy decreases as a function of the QD's radius for all potential barriers; and (iv) at critical value of the SQD radius limit two different potential barrier behaviors are obtained.

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