# Spatially Screening and Barrier Effects on Shallow Donor Binding Energy in $(In, Ga)N/GaN$ Cylindrical QWWs

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**Abstract:** In this paper, the ground-state binding energy of axial Hydrogenic sallow-donor impurity in $In_xGa_{1-x}N/GaN$ cylindrical quantum well wire (CQWWs) is calculated as a function of the wire radius within the effective mass approximation using a variational procedure. Spatially screening and potential barrier effects are investigated. Numerical results show that the binding energy is dramatically affected by the wire radius and the potential barrier. It is also affected by spatially screening phenomenon and its maximum moves to narrow wire.
**Keys word:** Binding Energy, Quantum well wire, Spatially Screening effect, Barrier effect
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## I. Introduction :

In the last few years, several experimental and theoretical works have been devoted to the quantitative understanding of the physical properties in particularly for $GaAs/(Ga, Al)As$ quantum wells (QWs), quantum-well wires (QWWs) and quantum dots (QDs) [1-6]. In the last few decades, wide-energy band gap III-V nitride semiconductors $GaN$, $AlN$ and $InN$, and their ternary alloys have received considerable attention. This considerable interest in the study of the physics underlying various properties of low-dimensional semiconductor systems is due to their importance for potential applications in electronic and optoelectronic devices, especially in blue and ultraviolet wavelengths. The binding energy of Hydrogenic impurities in these systems depends upon several micro (macro)-parameters such as semiconductor properties, impurities position and structural parameters (temperature, Hydrostatic pressure, electric and magnetic fields)$[7-14]$. To the best of our knowledge, no work has been done to treat the screening effect on the ground and excited-states binding energy of shallow donor impurity especially for $In_xGa_{1-x}N/GaN$ systems (QW, QWW, QD). For this reason, our results will be compared to those of others semiconductors such as $GaAs/Al_xGa_{1-x}As$ systems.

In this study, the spatially screening and barrier dependence of the ground-state shallow donor binding energy in $In_xGa_{1-x}N/GaN$ QWWs is calculated using a variational approach in the framework of the effective mass scheme.

## II. General formalism:

Shallow-donor impurity located at the center of the cylindrical quantum well wire (CQWW) of radius $R$, made out of $(In_xGa_{1-x}N)$ and Embedded in $GaN$ barrier is considered. In the framework of the effective mass approximation and restricting this study to the case which don't take account of the electron-phonon interaction and spin-orbit coupling, the hamiltonian of the system is given as follows :

$$H = -\frac{\hbar^2}{2m^*}\Delta + V_c(r) - \frac{e^2}{4\pi\varepsilon_0\varepsilon(r)r} \qquad (1)$$

Here: $m^*$ is the electron effective-mass in the $(In_xGa_{1-x}N)$ well the barrier (GaN) regions and $\varepsilon(r)$ is the spatially varying dielectric function. $V_c(r)$ represents the potential confinement which is assumed to be finite in the barrier. It is given as following:

$$V_c(r) = \begin{cases} 0 & r \le R \\ V_0 & elsewhere \end{cases} \qquad (2)$$

The trial function, in this case, is taken to be:

$$\Psi(\vec{r}) = Nexp\left[-\frac{\lambda}{R}|\vec{r}|\right]\begin{cases} J_0\left(\alpha_0\,\frac{r}{R}\right) & r \le R \\ \frac{J_0(\alpha_0)}{K_0(\beta_0)}K_0\left(\beta_0\,\frac{r}{R}\right) & r > R \end{cases} \qquad (3)$$

Here: $N$ is the normalization constant, $\lambda$ is the trial parameter, $J_0\left(\alpha_0\,\frac{r}{R}\right)$ is the zeroth order Bessel function and $K_0(\beta_0 r)$ is the zeroth order modified Bessel function. The exponential term describes the coulomb spatial interaction. The terms $\alpha_0$, $\beta_0$ and $|\vec{r}|$ are given by the formulas:

$$\alpha_0 = \frac{R}{\hbar}\sqrt{2m^*E_0}\,,\ \beta_0 = \frac{R}{\hbar}\sqrt{2m^*(V_0 - E_0)} \text{ and } |\vec{r}| = \sqrt{r^2 + z^2} \qquad (4)$$

Here: $V_0$ is the conductor band offset. Following the recent work of Schulz et al reported in Ref. [12], the band offset $\Delta E_c/\Delta E_v$ is taken to be $70:30$. Then, $V_0$ is given as:

 

$$V_0 = \frac{7.\Delta E_g}{10} \quad \text{and} \quad \Delta E_g = E_g(GaN) - E_g(In_xGa_{1-x}N) \tag{5}$$

The band structure of $(In, Ga)N$ ternary systems is calculated by use of Luttinger-Kohn $4 \times 4\vec{k}.\vec{P}$ Hamiltonian[15]. The band gap energy of $In_xGa_{1-x}N$ ternary alloy at room temperature is governed by the following formulas:

$$E_{g,InGaN}(x) = x.E_{g,InN} + (1-x).E_{g,GaN} - 1.43x(1-x) \text{ (eV)} \tag{6}$$

Where: $E_{g,InN}$ and $E_{g,GaN}$ are the band gap energies of $InN$ and $GaN$ at room temperature which are respectively equal to $0.77eV$ and $3.42eV$ [16,17].

The binding energy is obtained by minimization with respect to the trial parameter. It is given by :

$$E_b = E_0 - \underbrace{min}_{\lambda} \frac{<\psi(\vec{r})|H|\psi(\vec{r})>}{<\psi(\vec{r})|\psi(\vec{r})>} \tag{7}$$

Here: $E_0$ represents the electron state energy in the CQWW without the impurity.

In this study, we have used the Hermanson's model in which the spatially dielectric function is expressed as follows[18]:

$$\frac{1}{\varepsilon(r)} = \frac{1}{\varepsilon^*} + \left(1 - \frac{1}{\varepsilon^*}\right) \exp\left(-\frac{r}{c}\right) \tag{9}$$

Here: $\varepsilon^*$ is relative static dielectric constant and $c$ is the screening constant. Taken account of the results reported in [18] (page 3022), this later is chosen to be 0.9 (a. u).

The effective mass $m^*$ [19,20] and the relative static dielectric constant $\varepsilon^*$ [21] of $In_xGa_{1-x}N$ are expressed in the linear approximation as follow:

$$m^* = x.m^*_{InN} + (1-x).m^*_{GaN} \tag{10}$$

$$\varepsilon^* = x.\varepsilon^*_{InN} + (1-x).\varepsilon^*_{GaN} \tag{11}$$

For simplification, our results are given in the effective units $a^* = \frac{\varepsilon^*\hbar^2}{m^*e^2}$ ($2.70nm$ for $GaN$, $6.10nm$ for $InN$ and $2.80nm$ for $In_{0.2}Ga_{0.8}N$ ternary) and $R^* = \frac{m^*e^4}{2\varepsilon^*\hbar^2}$ (27.48meV for $GaN$, $12.22meV$ for $InN$ and $26.65meV$ for $In_{0.2}Ga_{0.8}N$ ternary).

**III. Results and discussion:**

In order to understand the spatially screening dependence of the shallow donor impurity binding energy, we have performed numerically computation for $In_xGa_{1-x}N/GaN$ QWWs structures. Figure 1 shows the results obtained for two Indium concentrations equal to $x = 0.2$ and $x = 0.4$ for a dielectric constant. One can see that the binding energy maximizes for all indium fraction and the maximum is obtained around $1.06nm$ ($R = 0.38$). When the wire radius is much larger than the effective Bohr radii (EBR), the electronic wave-function almost doesn't penetrate into the barriers and then the donor bending energy decreases as function of the wire radius increases and finally $(R \to \infty)$ tends to the $3D$ result, i.e., the effective Rydberg energy for $In_xGa_{1-x}N$ bulk material. With decreasing the wire radius, the quantum confinement size reduces and the binding energy increases and finally $(R \to 0)$ tends to an infinite value for an infinite QWWs barrier as expected theoretically by the formulas presented in Ref. [22]:

$$E_b = \frac{4R^*}{(2n+D-3)^2} \tag{12}$$

Where: $R^*$ is the effective Rydberg, $n$ is the principal quantum number and $D$ is the quantum confinement size; $(D = 1)$ for the QWWs.

However, in the finite potential barrier case as presented in this paper, the electronic wave-function cannot be confined completely in the well and partly penetrate into the barriers for the wire radius is getting narrower than the EBR of the impurity state and finally the binding energy does not reach to the $1D$ limit, but reasonably closes to the effective Rydberg $(R^*)$ when the wire becomes very much narrow $(R \to 0)$. At this point, one can affirm that the binding energy decrease for the narrow wire $(R < 1nm)$ can be explained by the wave-function expand across the barrier, i.e., the electron-impurity coverage distance increases. As expected, this expansion is governed by barrier height, i.e., by the indium fraction in the wire and then the binding energy is strongly affected by the barrier potential $(V_0(x))$. This effect is shown on figure 1 in which we have presented the results for two indium fraction in the wire. It is seen that for all wire radius the binding energy increases as a function of the indium concentration. This behavior can be explained by the In concentration dependence of the potential barrier. As the In concentration increases the band gap energy decreases which raises relatively the height of the potential barrier. This effect enhances the confinement of the impurity states resulting a higher binding energy. However, one can see that this increase is not uniform everywhere. It is the same for large and narrow wires but it is important and very significant around the maximum corresponding to the radius around the EBR. For very large wire the particle is away from the barriers; therefore it does not sense how the height of the potential barrier is. In the other extreme, the wire radius is so small that the particle cannot reside in the well, so it leaks out totally to the barrier and becomes insensitive to the potential barrier. It is shown also that the binding energy maximum moves slightly to narrow wire as a function of the In concentration. This is due to the fact that the EBR decreases as a function of the In concentration.

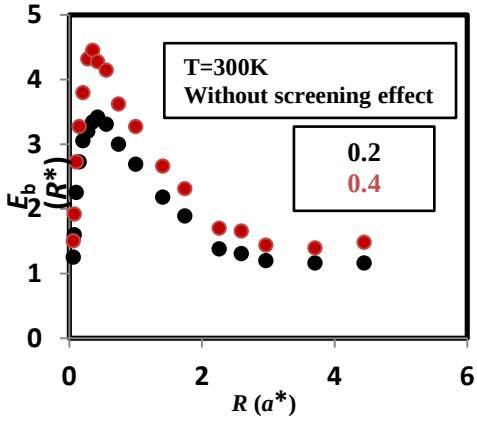


**Figure 1: Ground-state shallow donor binding energy as a function of the $In_xGa_{1-x}N/GaN$ CQWWs radius at room temperature without screening effect. The barrier effect is included.**

 

In Figure 2, the spatially screening effect on shallow donor binding energy is investigated as a function of the CQWWs radius. The Indium concentration and temperature are fixed respectively at $x = 0.2$ and $300K$. It is clear that the binding energy tends to the finite value as the radius becomes smaller and larger than the EBR. This behavior can be explained by the fact that the screening phenomenon disappears especially for the narrow and large wire which is in good agreement with Eq. (9). We should note that for the smaller distances $r \longrightarrow 0$, $\varepsilon(r) \longrightarrow 1$ and for the larger distances $(r \gg c)$ the screening becomes constant $(\varepsilon(r) \longrightarrow \varepsilon^*(x = 0.2))$. It has found also that the screening effect is more pronounced for the wire radius around $1nm$. The maxima are obtained at $1.06nm$ $(R = 0.38)$ and $0.91nm$ $(R = 0.32)$ for the constant dielectric and the Hermanson's model respectively. These results show that the maximum of the binding energy moves to narrow wire as a function of the screening effect. This displacement is about 14%. It is apparent that the spatially screening effect is the same as that of the In concentration. This is due to the fact that as the In concentration increases the spatially screening effect increases too. It is also obtained that the spatially screening effect induces a displacement of the binding energy maximum to the narrow wire. This result is in good agreement with that of the In concentration which is pointed out before. Therefore, this shift can be attributed to the dependence of the EBR as a function of the spatially screening, i.e. as the In concentration increases the spatially screening increases too and the EBR decreases.

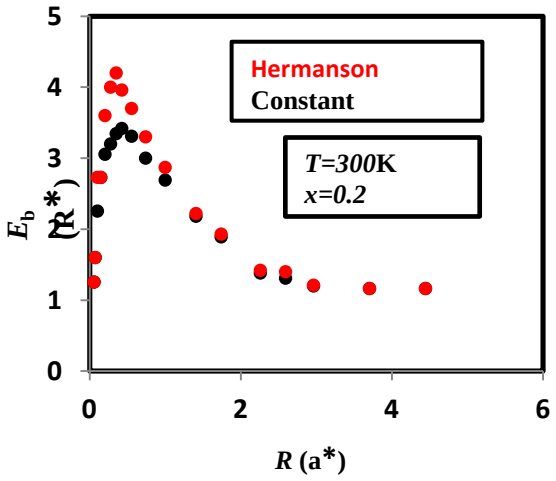


**Figure 2: The ground-state shallow donor binding energy as a function of $In_{0.2}Ga_{0.8}N/GaN$ QWW radius at room temperature. The screening effect is included.**

Our results are in good agreement with those reported by different authors in the literature in particularly for $GaAs/Al_xGa_{1-x}As$ systems. For example, the authors of references [5, 23] for cylindrical and square QWWs, [24] for spherical quantum dot (SQD) and [25] for the quantum well, have shown that the screening effect increases the binding energy and this increase depends of the well dimension. It is more pronounced around the maximum and diminishes for larger and narrower well. On the other hand, the results reported by Peter et al [18] concerning the $QD$ under different confinement such as parabolic, spherical and rectangular aren't in good agreement with our results. They have shown that when the dielectric function is included in the potential term, the binding energy decreases for all the dot radii (Fig.3 in [18]). This behavior is due probably to the applied electric field which is $10^5 V.cm^{-1}$ contrary to our results and those cited above which corresponds to the case without the electric field.

**Conclusion:**

The ground-state shallow donor impurity binding energy in $In_xGa_{1-x}N$ CQWWs is investigated numerically using variational procedure within the effective mass scheme. The spatially dependence of the dielectric function, wire radius and potential height are taking account. The results reveal that the binding energy:

- Increases for all $CQWW$ radii.
- Maximizes and moves to the narrow wire under spatially screening and potential barrier effects.

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