Influence of Pressure on the Binding Energy of Two Donors in a Strained Zinc Blende GaN/AlGaN Quantum Dot

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Abstract: The binding energy two donors in a strained GaN/Al\textsubscript{\textit{x}}Ga\textsubscript{1-x}N spherical quantum dot (SQD) are calculated using a variational method based on the single band effective mass approximation. The binding energy of two donors is computed as a function of quantum dot size and hydrostatic pressure. The numerical results show that the binding energy increases with the pressure for any size of dot. We compare the binding energy of two donors with and without strain effects, and the results show that the strain effects enhance the impurity binding energy considerably, especially for the small quantum size. Our results are good in agreement with existing literatures.

Keywords: Strained Quantum Dot, Variational Method, Hydrostatic Pressure

1. Introduction

Recently, Studies on group III nitrides and related nanostructures attract significant attention as promising candidates for application in optical, electronic and optoelectronic devices. Growth in GaN technology has led to many reports on fabrication and characterization of different kinds of GaN QDs [1–4]. The wide band gap group III nitrides exist in two structural phases such as wurtzite and zinc blende structural phases [5]. The physical properties of wurtzite phase nitride structure are highly affected by the strong built-in electric fields due to the spontaneous and piezoelectric polarizations [6]. In contrast, these spontaneous and piezoelectric polarizations can be negligible in zinc blende nitride structures, due to the high crystal symmetry of ZB phase [7]. In addition to that, the energy gap of the ZB III nitrides is smaller than that of their WZ counterparts [8]. It shows that zinc blende nitrides and related nanostructures exhibit superior electronic and optical properties over its wurtzite counterparts [9,10].

For the past few decades, much theoretical and experimental work have been devoted in investigating electronic structure and binding energy of a hydrogenic impurity in different shape QDs [11,12] with different external perturbations such as applied electric field, magnetic field and pressure[13-15]. These results revealed that the external perturbations influence greatly the impurity states, the electronic mobility and the optical properties of low dimensional semiconductor structures. Among the various external perturbations, hydrostatic pressure can shift effectively the energy levels of semiconductor nanostructures without altering the crystal symmetry. Because the applied pressure can also alter the strain effects, it has fascinated considerable attention both theoretically and experimentally [16-18].

However, there are many authors reported the impurity states in GaN/AlGaN ZB QDs. More recently, acceptor and donor impurities in GaN nanocrystals have been reported [19]. We have also studied the hydrogenic donor impurity states in ZB GaN-based QDs [20].
Although many authors have discussed the impurity states in GaN/Al\textsubscript{x}Ga\textsubscript{1-x}N zinc blende QDs \cite{21, 22}, the strain and pressure are neglected in previous works. Thus, further research is meaningful to the design and manufacture of optoelectronic devices. In this paper, we investigate the effects of hydrostatic pressure on the binding energy of two donor impurity in a strained GaN/Al\textsubscript{x}Ga\textsubscript{1-x}N spherical finite-potential ZB QD using the variational approach with the effective mass approximation. Our results seem to be more reliable than those obtained before \cite{23, 24}, since the influence of strain due to the mismatch of lattice constants are considered here.

2. Theory and Model

Within the framework of effective-mass approximation, the Hamiltonian for a heliogenic impurity in the cylindrical ZB GaN/GaAlN QD, under the influence of the hydrostatic pressure along the growth direction, may be written as

\[ H = H_0 - \frac{e^2}{4\pi\varepsilon_0\varepsilon(P)|\vec{r}_1 - \vec{r}_2|} \]  

(1)

With

\[ H_0 = \sum_{j=1}^{2}\left[ \frac{1}{2m^*}\left( \vec{p}_j + \frac{e A_j}{c} \right)^2 + V_D(\vec{r}_j) \right] \]  

(2)

where \( V_D = \frac{V_{ob}r^2}{R^2} \) for \( |r| \leq R \) and \( V_D = V_{ob} \) for \( |r| > R \). \( V_{ob}(\vec{r}) \) is the barrier height given by \( V_{ob}(\vec{r}) = Q_c\Delta E_g(x) \). \( Q_c \) is the conduction band off-set parameter, which is taken to be 70% of the conduction band and \( m^* \) is the effective mass of the electron which is equivalent to 0.19\( m_e \) and \( \varepsilon_o\) is the effective dielectric constant of the quantum dot, and \( \varepsilon(P) \) is the pressure-dependent effective mean relative dielectric constant of the zinc blende GaN material.

Due to the mismatch of lattice constants and applied hydrostatic pressure, we consider the variations of parameters, such as dot size, dielectric constant and effective mass. The donor binding energy is affected by the variations. In present paper, we display the above parameters of GaN and AlN depends on strain and hydrostatic pressure. The corresponding parameter of Al\textsubscript{x}Ga\textsubscript{1-x}N can be obtained by linear interpolation method \cite{25}.

The pressure dependent lattice constant is expressed by Murnaghan state equation \cite{26}:

\[ a_j(P) = a_j(0)\left[ 1 - \frac{P}{3B_{oj}} \right] \]  

(3)

Where \( a_j(0) \) is the \( j \) material’s lattice constant for zero pressure, and \( B_{oj} \) is the \( j \) material’s bulk modulus of zinc-blende structure.

The variations of biaxial and uniaxial strain tensor ratio with pressure can be written as \cite{27}

\[ \epsilon_{xx,j}(P) = \epsilon_{yy,j}(P) = \frac{a_k(P) - a_j(P)}{a_j(P)} \]  

(4)

\[ \epsilon_{zz,j}(P) = -2\frac{C_{12,j}}{C_{11,j}} \epsilon_{xx,j}(P) \]  

(5)

Where \( j \) is GaN (Al\textsubscript{x}Ga\textsubscript{1-x}N) material, \( k \) is Al\textsubscript{x}Ga\textsubscript{1-x}N (GaN) material, and \( C_{11,j} \) and \( C_{12,j} \) are elastic constants for \( j \) material.

The hydrostatic pressure \( P \) dependent band gap is given as \cite{26}

\[ E_{g,j}(P) = E_{g,j}(0) + bP + cP^2 \]  

(6)
Where \(b\) and \(c\) are the pressure coefficient of band gap for GaN or Al\(_{1-x}\)Ga\(_x\)N, and the band gap of Al\(_{1-x}\)Ga\(_x\)N for zero pressure obtained by linear interpolation method.

In the strained zinc blende GaN quantum dot, the variation of band gap with the pressure and strain can be considered as [27]

\[
E_{g,j}(P, \epsilon) = E_{g,j}(P) + (\alpha_j^c - \alpha_j^v)\left[2\varepsilon_{xx,j}(P) + \varepsilon_{zz,j}(P)\right]
\]  
(7)

Where \(\alpha_j^c\) and \(\alpha_j^v\) are the deformation potentials of conduction and valence band, respectively.

The pressure and strain dependent electronic effective mass is given by [28]

\[
\frac{m_j}{m_j} = 1 + \frac{C_j}{E_{g,j}(P, \epsilon)}
\]  
(8)

Where \(C_j\) is a constant and can be determined by solving Equation (9) when \(P=0\). The hydrostatic pressure dependence of frequencies can be written by the Gruneisen parameter [26].

\[
\gamma_j = B_{0,j} \frac{1}{\omega_{\nu,j}} \frac{\partial \omega_{\nu,j}(P)}{\partial P} \quad [i = \text{LO, TO}]
\]  
(9)

The modified phonon energy due to pressure can be written as

\[
h\omega_{\nu,j}(P) = h\omega_{\nu,j}\exp\left(\frac{r_{\nu,j}}{B_{0,j}}P\right) \quad [i = \text{LO, TO}]
\]  
(10)

The hydrostatic pressure dependence of high frequency dielectric constant can be written as [29]

\[
\varepsilon_{\nu,j}(P) = 1 + \left[\varepsilon_{\nu,j} - 1\right]\exp\left[\frac{5}{3B_{0,j}}(f_{\text{ion,j}} - 0.9)P\right]
\]  
(11)

Using the Lyddane-Sachs-Teller (LST) relationship [27], the static-dielectric constant with pressure effect can be given as

\[
\varepsilon_{0,j}(P) = \varepsilon_{\nu,j}(P)\left[\frac{h\omega_{\nu,0}}{h\omega_{\nu,0}}\right]^2
\]  
(12)

Using the linear interpolation method, the other parameters with pressure for ternary mixed crystal Al\(_{1-x}\)Ga\(_x\)N can be obtained as follows

\[
Q_{Al_{1-x}Ga_xN} = (1-x)Q_{GaN} - xQ_{AlN}
\]  
(13)

Where \(Q_{GaN}\) and \(Q_{AlN}\) are the corresponding parameters associated with GaN and AlN, respectively.

In order to calculate the ground state binding energy of two donor impurities in ZB GaN/AlGaN QD, the trial wave function may be written as

\[
\Psi_{1,2}(\vec{r}_1, \vec{r}_2) = \left\{
\begin{array}{l}
N_1 \frac{\sin(\alpha_{1,r})}{r} e^{-\gamma r_1} e^{-\xi_1 r_1} e^{-\xi_2 r_2}, \\
N_2 \frac{e^{-\beta_{1,r}}}{r} e^{-\gamma r_2} e^{-\xi_1 r_1} e^{-\xi_2 r_2}
\end{array}
\right.
\]  
(14)

Where \(\gamma\), \(\xi_1\) and \(\xi_2\) are the variational parameter.
The confining potential energies of two interacting donors are calculated using the wave functions

Equation (14) for 1s states is obtained by,

\[ H_{1e} = \left\langle \Psi_1 (\vec{r}_1, \vec{r}_2) \right| \frac{2}{|\vec{r}_1 - \vec{r}_2|} \left| \Psi_1 (\vec{r}_1, \vec{r}_2) \right\rangle \]  
(15)

In the above equation \(|\vec{r}_1 - \vec{r}_2|\) determines the role of inter donor distances in the Coulomb interaction energy of two donor systems.

The ground state energy of two donor impurities in ZB GaN/AlGaN QD, may be obtained by minimizing

\[ E = \min_{\vec{r}, \vec{r}'} \frac{\langle \Psi_1 (\vec{r}, \vec{r}) \rangle H |\Psi_1 (\vec{r}, \vec{r})\rangle}{\langle \Psi_1 (\vec{r}, \vec{r}) \rangle |\Psi_1 (\vec{r}, \vec{r})\rangle} \]  
(16)

The ground state binding energy of two donors \(E_b\) can be obtained as follows

\[ E_b = E_0 - E \]  
(17)

Where \(E_0\) is the ground state energy for the Hamiltonian of equation (2).

3. Results and Discussion

In order to study the pressure and strain dependences of the binding energy of two donors, we perform numerical computation for GaN/Al\(_x\)Ga\(_{1-x}\)N spherical QD within the framework of effective mass approximation. Using the band gap difference [30] of \(E_{g, AlGaN} = E_g,GaN(1-x) + xE_g,AlN + 530(1-x)x\) (meV) and assuming 70% contribution to the conduction band, the value of \(V_0\) is \(V_0=0.6 (E_{g, AlGaN} - E_g,GaN)\). The parameters used in the computations are got from Refs. [26, 31-33]. The calculated results are presented in Figures 1-4.

The character of the sub-band energy dependence on pressure varies with the QD radius as illustrated in Figure 1. As we expected, the sub-band energy increases with squeezing the radius of the dot with and without the influence of pressure. Also we observed that the sub-band energy have more influence for narrow dots irrespective of the applied pressure. Due to influence of pressure, the size of the quantum dot is reduced which increases the sub-band energy of the confined electron.

![Figure 1. Sub-band energy with dot radius for different Pressure](image-url)
In Figure 2, the ground state binding energy of two donors in the strained ZB GaN quantum dot is calculated as a function of dot radius and different hydrostatic pressures $P = 0$ GPa, $P = 10$ GPa and $P = 20$ GPa. It is found that the binding energy increases with a decrease of dot radius, reaching a maximum value and then decreases when the dot radius still decreases. This is a common feature in all quantum heterostructures. The confining potential has very small influence on the impurity state when the dot radius is extremely large, and therefore it tends to the free electron case and the binding energy trends to a constant value. For a smaller dot radius, one has a $\delta$ function potential with a finite strength, and tunneling effects are enhanced. Hence, the binding energy attains a maximum value [24, 34].

Moreover, it is also observed that the hydrostatic pressure increases the donor binding energy of the impurity. It is explained by the fact that the size of the QD is decreased when the hydrostatic pressure is applied. Then, the distance between the electron and the impurity is decreased when the hydrostatic pressure is increased. Thus, the binding energy of two donors is increased as a result of the increasing of the Coulomb interaction between the electron and impurity when the hydrostatic pressure is considered. On the other hand, we found that the influence of pressure is more appreciable for the small dot sizes as shown in Figure 2a, which is in good agreement with C.X. Xia [18].

The ground-state binding energy of two donors is investigated as a function of the hydrostatic pressure in strained ZB GaN/AlGaN QD for different dot radius as shown in Figure 3. It is found that the donor binding energy increases linearly when the hydrostatic pressure increases. This is because the electron is much more localized inside the strained ZB GaN QD when the hydrostatic pressure is increased. It shows that the Coulomb interaction between the electron and the impurity, donor binding energy increase with increasing the hydrostatic pressure. In particular, from Figure 3 also shows that the donor binding energy is much more sensitive to the hydrostatic pressure when the dot size is small.

![Figure 2. Binding energy with dot radius as a function of different hydrostatic pressure](image-url)
Figure 2a. Binding energy with dot radius as a function of different hydrostatic pressure

Figure 3. Binding energy as a function of pressure for different dot radius

In Figure 4, the Coulomb interaction energy of two donors is calculated as a function of pressure for different dot radius with a constant inter-donor distance ($r_1 - r_2 = 50 \text{ Å}$). It is found that the interaction energy significantly increases the donor binding energy. We also observed that the Coulomb interaction energy increases linearly when the pressure is applied. It is shown that the interaction energy strongly depends on inter donor distances and the interaction energy is appreciable when approaching the inter donor distances.
5. Conclusion

In conclusion, the binding energy of two donors in a strained zinc-blende GaN/Al,Ga1-xN spherical QD is discussed with a variational method by considering the influence of hydrostatic pressure. The results show that the binding energy of two donor impurities increases with pressure for any dot radius. In addition, our results also show that the Coulomb interaction energy is increased linearly when the hydrostatic pressure is increased. The influence of strain effects on the binding energy for small dot radius is stronger than that for large dot radius. We also hope that our results can stimulate further investigations of the related physics, as well as device applications in strained ZB GaN/AlGaN QD.

References

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