Barrier Thickness and Hydrostatic Pressure Effects on Hydrogenic Impurity States in Wurtzite GaN/Al\textsubscript{x}Ga\textsubscript{1-x}N Strained Quantum Dots

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Received 6 January 2015; Accepted 17 March 2015

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Within the framework of the effective mass approximation, barrier thickness and hydrostatic pressure effects on the ground-state binding energy of hydrogenic impurity are investigated in wurtzite (WZ) GaN/Al\textsubscript{x}Ga\textsubscript{1-x}N strained quantum dots (QDs) by means of a variational approach. The hydrostatic pressure dependence of physical parameters such as electron effective mass, energy band gaps, lattice constants, and dielectric constants is considered in the calculations. Numerical results show that the donor binding energy for any impurity position increases when the hydrostatic pressure increases. The donor binding energy for the impurity located at the central of the QD increases firstly and then begins to drop quickly with the decrease of QD radius (height) in strong built-in electric fields. Moreover, the influence of barrier thickness along the QD growth direction and Al concentration on donor binding energy is also investigated. In addition, we also found that impurity positions have great influence on the donor binding energy.

1. Introduction

Recently, much attention has been paid to wide-band gap wurtzite (WZ) GaN/AlGaN quantum heterostructures due to their promising applications in optoelectronic devices such as light-emitting devices (LEDs) and laser diodes (LDs) [1–3]. Doping impurities in GaN-based confined systems is an effective method for controlling the electronic and optical properties of optoelectronic devices. It is well known that the hydrostatic pressure applied on a GaN-based semiconductor material can not only modify the parameters, such as the band gaps, the potential barriers, the conduction effective masses, the static dielectric constants, and the lattice constants, but also change the dimension of the low-dimensional systems, which is associated with the fractional change in the volume. Moreover, the strong built-in electric field induced by the spontaneous and piezoelectric polarizations also affects obviously the distribution of the carrier wave function in WZ nitride-based quantum heterostructures. According to the above characteristics, various studies concerning impurity states are reported in GaN-based nanostructures such as quantum wells [4–8], quantum well wires [9, 10], and (double) quantum dots [11–17]. In these references, considering the strong built-in electric field and/or hydrostatic pressure effects, the hydrogenic donor impurity states are mainly discussed in a radial infinite confinement potential barrier. Their results demonstrate that quantum structure size, strong built-in electric field, and hydrostatic pressure have a significant influence on the donor impurity binding energies, but there are few reports involved in barrier thickness effects on the donor binding energy in WZ GaN/Al\textsubscript{x}Ga\textsubscript{1-x}N strained QD in finite potential barrier to date.

To further demonstrate the barrier thickness effect on impurity states in a WZ GaN/AlGaN strained QD, we calculate the donor binding energy of hydrogenic impurity in a WZ GaN/AlGaN QD under a strong built-in electric field by means of a variational approach in the finite confinement potential. In our calculation, effective mass of the electron, dielectric constants, phonon frequencies, energy gaps, sizes
Figure 1: The diagram of a cylindrical wurtzite GaN/Al\(_x\)Ga\(_{1-x}\)N QD.

(radius and height) of QD, and piezoelectric polarizations are considered as a function of hydrostatic pressure. The paper is organized as follows. In Section 2, we describe the theoretical framework. Then, the pressure and the strain coefficients of GaN and Al\(_x\)Ga\(_{1-x}\)N are discussed in Section 3. In Section 4, the numerical results are discussed. Finally, conclusions are drawn from the present study in Section 5.

2. Theoretical Framework

In Figure 1, the schematic view of a cylindrical WZ GaN/Al\(_x\)Ga\(_{1-x}\)N QD is depicted, with a detailed description of the different dimensions of the QD (dot radius \(R\), height \(L_w\), and barrier thickness \(L_b\)). Additionally, the GaN quantum dot is embedded in an Al\(_x\)Ga\(_{1-x}\)N host matrix material, and the \(z\)-axis is defined to be the growth direction. Within the frame of the effective mass approximation, the Hamiltonian for a hydrogenic donor impurity in cylindrical WZ GaN/Al\(_x\)Ga\(_{1-x}\)N QD under the influence of hydrostatic pressure can be written [4] as

\[
\tilde{H} = \tilde{H}_0 - \frac{\hbar^2}{4\pi\varepsilon_0 \tilde{e}(p)} \left( \frac{\hbar^2}{\tilde{e}^2} \right) \left( \frac{\hbar^2}{\tilde{e}^2} \right),
\]

where \(\tilde{r}(\tilde{r}_0)\) denotes the position vector of the electron (impurity ion), \(\varepsilon\) is the absolute value of the electron charge, \(\varepsilon_0\) is the permittivity of free space, and \(\tilde{e}(p)\) is the pressure-dependent effective mean relative dielectric constant of GaN and Al\(_x\)Ga\(_{1-x}\)N materials. The Hamiltonian \(\tilde{H}_0\) is given by [11]

\[
\tilde{H}_0 = -\frac{\hbar^2}{2m_\perp(p)} \left( \frac{\hbar^2}{\tilde{e}^2} \right) \left( \frac{\hbar^2}{\tilde{e}^2} \right) - \frac{\hbar^2}{2m_\parallel(p)} \frac{\partial^2}{\partial z^2} + V(\rho, z, \rho) + eF_{wb}(\rho) z,
\]

where \(m_\perp\) and \(m_\parallel\) are the pressure- and strain-dependent effective masses of electron along and perpendicular to the [0001]-direction. And \(V(\rho, z, \rho)\) is the electron confinement potential due to the band offset \((Q_f = 0.765)\) and is given by [13]

\[
V(z, \rho) = \begin{cases} Q_f \left[ E_{g, Al, Ga_{1-x}N} - E_{g, GaN} \right], & 0 < z < \frac{L_w}{2} + \frac{L_b}{2} \\ -\frac{L_w}{2} - \frac{L_b}{2} < z < -\frac{L_w}{2}, & |z| \leq \frac{L_w}{2}, \end{cases}
\]

(3)

\[
V(\rho, \rho) = \begin{cases} 0, & \rho \leq R, \\ Q_f \left[ E_{g, Al, Ga_{1-x}N} - E_{g, GaN} \right], & \text{others.} \end{cases}
\]

(4)

In (2), \(f(p)\) is the pressure-dependent built-in electric field (BEF) in the finitely thick barrier layer for WZ GaN/Al\(_x\)Ga\(_{1-x}\)N QD. The values of the BEF along the growth direction in the well \((F_{GaN})\) and barrier \((F_{Al, Ga_{1-x}N})\) that result from the difference in the total electric polarizations in each region are given by simple formulas [14]:

\[
F_{GaN}(p) = -\frac{L_w}{L_b} F_{GaN}(p),
\]

(5)

where \(L_w, L_b\) and \(\varepsilon_{GaN}^{Al}, \varepsilon_{GaN}^{Al}\) are the thicknesses and electronic dielectric constants for GaN and Al\(_x\)Ga\(_{1-x}\)N materials, \(P_{sp}^{GaN}, P_{sp}^{Al}\) and \(P_{pe}^{GaN}, P_{pe}^{Al}\) are the spontaneous and piezoelectric polarizations for GaN and Al\(_x\)Ga\(_{1-x}\)N materials, and the bowing parameter \(\eta\) is chosen as \(-0.019\) C/m\(^2\) [14]:

\[
P_{sp}^{Al} = x P_{sp}^{Al} + (1 - x) P_{sp}^{GaN} - \eta x (1 - x).
\]

(6)

The wave function of the electron confined in the WZ GaN/Al\(_x\)Ga\(_{1-x}\)N QD can be written as

\[
\psi(\rho, \varphi, z) = f(\rho) h(z)e^{im\varphi}, \quad m = 0, \pm 1, \pm 2, \ldots,
\]

(7)

\[
f(\rho) = \begin{cases} I_0(\beta \rho), & \rho \leq R, \\ K_0(\beta R) K_0(\alpha \rho), & \rho > R, \end{cases}
\]

where the constants \((\alpha, \beta)\) are determined by the continuity of the derivative of the radial wave function at the QD boundary and \(m\) is the electron \(z\)-component angular momentum quantum number. The radial wave function \(f(\rho)\) of the electron can be obtained using the Bessel function \(I_m\)
and the modified Bessel function $K_{m'}$. Wave function $h(z)$ can be expressed by means of the Airy functions $Ai$ and $Bi$ [16]:

$$
h(z) = \begin{cases} 
C_1 Ai(\epsilon_1) + D_1 Bi(\epsilon_1) & \frac{L_w}{2} - L_b < z < -\frac{L_w}{2}, \\
C_2 Ai(\epsilon_2) + D_2 Bi(\epsilon_2) & |z| \leq \frac{L_w}{2}, \\
C_3 Ai(\epsilon_3) + D_3 Bi(\epsilon_3) & \frac{L_w}{2} < z < \frac{L_w}{2} + L_b.
\end{cases}
$$

(8)

Here $\epsilon_j = ((2m_j^*/\hbar^2)EF)^{1/3} (z - E_z - V(z, p))/EF$. The coefficients $C_j$ and $D_j$ ($j = 1, 2, 3$) can also be obtained by the transfer matrix methods [16].

In order to calculate the donor binding energy, the trial wave function can be chosen as [17]

$$
\phi(\rho, \varphi, z) = N \psi(\rho, \varphi, z) e^{-\alpha(\rho - \rho_0)^2 - \beta (z - z_0)^2},
$$

(9)

where $N$ denotes the normalization constant; with the adiabatic approximation, the donor binding energy of a hydrogenic impurity $E_b$ is defined as the difference between the ground-state energy of the system without impurity and the ground-state energy of the system with impurity; that is,

$$
E_b = E_{0\rho} + E_{0z} - \min_{\alpha, \beta} \langle \psi | H | \psi \rangle.
$$

(10)

### 3. Pressure and Strain Dependence of Physical Parameters

In this model, we take the strains induced by the biaxial lattice mismatch into account. The components of biaxial stress tensors of GaN and AlGaN materials are given under lattice mismatch into account. The components of biaxial stress tensors of GaN and AlGaN materials under hydrostatic pressure $P$ [18]:

$$
\epsilon_{xx, \text{Ga}N} = \epsilon_{yy, \text{Ga}N} = \frac{a_{eq}(P) - a_{\text{Ga}N}(P)}{a_{\text{Ga}N}(P)},
$$

$$
\epsilon_{xx, \text{Al}GaN} = \epsilon_{yy, \text{Al}GaN} = \frac{a_{eq}(P) - a_{\text{Al}GaN}(P)}{a_{\text{Al}GaN}(P)},
$$

(11)

where the equilibrium lattice constant $a_{eq}$ for the strained layer under hydrostatic pressure $P$ depends on the lattice constants of the component materials and is weighted by their relative thicknesses [19]:

$$
a_{eq}(P) = a_{\text{Ga}N} \frac{L_w + a_{\text{Al}GaN} L_b}{L_w + L_b}.
$$

(12)

The lattice constant $a_e$ of the GaN (AlN) material dependence of hydrostatic pressure satisfies [20]

$$
a_e(P) = a_{0\nu} \left( 1 - \frac{P}{3 \beta_{0\nu}} \right), \quad \nu = \text{GaN, AlN}.
$$

(13)

Here the actual lattice constant $a_{\text{Al}GaN}$ of the Al$_{1-x}$Ga$_x$N material can be obtained by the linear interpolation method from the corresponding values of GaN and AlN. $L_{\text{Ga}N}(L_{\text{Al}GaN})$ is the thickness of the dot (barrier) layer. The strain induced by the biaxial lattice mismatch along the $z$-direction in the heterostructure is [21]

$$
\epsilon_{zz, \text{Ga}N} = \frac{R_{11\nu}}{m_{11\nu}^0} \epsilon_{xx, \text{Ga}N},
$$

$$
\epsilon_{zz, \text{Al}GaN} = \frac{R_{11\nu}}{m_{11\nu}^0} \epsilon_{xx, \text{Al}GaN}.
$$

(14)

The coefficient $R_{11\nu}$ of the GaN (AlN) material is given by [21]

$$
R_{11\nu} = \frac{C_{11\nu}(P) + 2C_{12\nu}(P) - 2C_{13\nu}(P)}{C_{33\nu}(P) - C_{13\nu}(P)}, \quad \nu = \text{GaN, AlN},
$$

(15)

where $C_{j\nu}$ is the pressure-dependent elastic stiffness constant of material $\nu$ and is given by [21] $C_{j\nu}=C_{j\nu}(0) + \alpha_{j\nu} P + \delta_{j\nu} P^2$ and the coefficient $R_{11\nu}$ and the pressure-dependent elastic stiffness constant $C_{j\nu}$ of Al$_{1-x}$Ga$_x$N material can be obtained by the linear interpolation method from the corresponding values of GaN and AlN. The strain-dependent energy gaps of GaN and AlN are [22]

$$
E_{g, \text{Ga}N} = E_{g, \text{Ga}N}(P) + 2 (a_{1\nu, \text{Ga}N} + b_{1\nu, \text{Ga}N}) \epsilon_{xx, \text{Ga}N} + (a_{2\nu, \text{Ga}N} + b_{2\nu, \text{Ga}N}) \epsilon_{zz, \text{Ga}N},
$$

$$
E_{g, \text{Al}GaN} = E_{g, \text{Al}GaN}(P) + 2 (a_{1\nu, \text{Al}GaN} \epsilon_{xx, \text{Al}GaN} + a_{2\nu, \text{Al}GaN} \epsilon_{zz, \text{Al}GaN},
$$

(16)

where $a_{1\nu}, a_{2\nu}, b_{1\nu},$ and $b_{2\nu} (\nu = \text{GaN and AlN})$ are the deformation potentials. The energy gap $E_{g, \nu}(P)$ dependence of hydrostatic pressure $P$ is considered by the following equation [22]:

$$
E_{g, \nu}(P) = E_{g, \nu}(0) + \chi_{\nu} P.
$$

(17)

The energy gap of the Al$_{1-x}$Ga$_x$N alloy can be calculated by the following formula [14]:

$$
E_{g, \text{Al}GaN}(P) = (1 - x) E_{g, \text{Ga}N} + x E_{g, \text{Al}N} - bx (1 - x).
$$

(18)

The biaxial strain and hydrostatic pressure dependences of the electron effective masses in the $x$-$y$ plane and the $z$-direction can be calculated by [23]

$$
\frac{m_0}{m_{11\nu}^0(P)} = 1 + \frac{C_{j\nu}}{E_{g, \nu}(P)},
$$

(19)

where $C_{j\nu}$ is a fixed value for a given material $\nu$ and can be derived from the values of $m_{11\nu}^0(0)$ and $E_{g, \nu}(0)$. In (5), under consideration of the biaxial strain in a wurtzite structure modified by hydrostatic pressure, the dielectric constants and the phonon eigen-frequencies will also change. The static dielectric constant $\epsilon_{\nu}$ is influenced by biaxial strain and hydrostatic pressure. The tensor components of $\epsilon_{\nu}$ for the WZ structure are derived from the generalized Lyddane-Sachs-Teller relation [24]:

$$
\epsilon_{\nu}^z(q) = \epsilon_{\nu}^{z'}(q) \left( \frac{\omega_{\text{TO}}^z(q)}{\omega_{\text{LO}}^z(q)} \right)^2,
$$

(20)
where the LO- and TO-phonon frequencies influenced by biaxial strain and hydrostatic pressure can be written as

\[
\omega_{j,k}^\nu = \omega_{j,k}^\nu (p) + 2K_{j,k,x}^\nu \varepsilon_{xx}^\nu (p) + K_{j,k,z}^\nu \varepsilon_{zz}^\nu (p).
\]  (21)

Furthermore, the hydrostatic pressure dependence of \( \omega_{j,k}^\nu \) can be given by [25]

\[
y_{j,k}^\nu = B_{0,\nu} \frac{1}{\omega_{j,k}^\nu (0)} \left( \frac{\partial \omega_{j,k}^\nu (p)}{\partial p} \right).
\]  (22)

where the subscript \( j \) represents LO or TO phonon, \( \xi (\xi = \perp \text{ or } z) \) denotes \( x \text{-}y \text{ plane or } z \text{-direction} \), \( \omega_{j,k}^\nu (0) \) is the zone-center phonon frequency of material \( \nu \), \( y_{j,k}^\nu \) is Gruneisen parameter of phonon mode given in [25], \( B_{0,\nu} \) is bulk modulus, and \( K_{j,k,xx}^\nu \) and \( K_{j,k,zz}^\nu \) are the strain coefficients of zone-center phonon modes. Following [14], the influence of hydrostatic pressure on the donor binding energy of hydrogenic impurity are investigated in WZ GaN/Al

\[
\frac{\partial \epsilon_{0,xx}^\nu (p)}{\partial p} = -\frac{5}{3} \epsilon_{0,xx}^\nu (0) (0.9 - f_{i0}^\nu).
\]  (23)

Here \( f_{i0}^\nu (\nu = \text{GaN and AlN}) \) is Phillips ionicity parameter of material; the static bulk modulus \( B_{0,\nu} \) under hydrostatic pressure is given by [25]

\[
B_{0,\nu} = \left( C_{11,\nu} (P) + C_{12,\nu} (P) C_{33,\nu} (P) - 2C_{13,\nu} (P) \right) C_{11,\nu} (P) + C_{12,\nu} (P) + 2C_{33,\nu} (P) - 4C_{13,\nu} (P) \)  \]  (24)

where \( C_{11,\nu}, C_{12,\nu}, C_{13,\nu}, \text{ and } C_{33,\nu} \) are the elastic constants of material \( \nu \). The effective mean relative dielectric constant in (I) is defined as [26]

\[
\mathcal{F}_{\nu} (p) = \frac{2}{3} \epsilon_{0,\perp}^\nu (p) + \frac{1}{3} \epsilon_{0,z}^\nu (p).
\]  (25)

Then the hydrostatic-pressure-modified biaxial and uniaxial strain dependence of the static dielectric constant is fully considered, whereas the dielectric constant of Al\(_{1-x}\)Ga\(_x\)-N can be calculated by the SCPA [13]. The piezoelectric polarization along the [0001] oriented WZ GaN/Al\(_x\)Ga\(_{1-x}\)-N QD can be calculated as [27]

\[
P_{PS} = e_{33}^\nu (p) \varepsilon_{xx}^\nu + 2e_{31}^\nu (p) \varepsilon_{xx}^\nu .
\]  (26)

where \( e_{31}^\nu \) and \( e_{33}^\nu \) are the pressure-dependent piezoelectric constants of material \( \nu \).

4. Results and Discussions

Under the strong built-in electric field induced by the spontaneous and piezoelectric polarizations, barrier thickness and hydrostatic pressure effects on the donor binding energy of hydrogenic impurity are investigated in WZ GaN/Al\(_x\)Ga\(_{1-x}\)-N strained QD. All material parameters used in our calculations are listed in Tables 1–4. Material parameters of Al\(_x\)Ga\(_{1-x}\)-N are estimated using a linear interpolation between the values of the corresponding parameters of GaN and AlN.
Table 1: Lattice constant $a$ (in units of nm), effective mass $m_e$ (in units of a free-electron mass $m_0$), piezoelectric constants $\varepsilon_{31}$ and $\varepsilon_{33}$ (in units of C/m²), and deformation potentials $a_1$, $a_2$, $b_1$, and $b_2$ (in units of eV) for GaN and AlN.

<table>
<thead>
<tr>
<th></th>
<th>$a$</th>
<th>$m_e$</th>
<th>$m_f$</th>
<th>$\varepsilon_{31}$</th>
<th>$\varepsilon_{33}$</th>
<th>$a_1$</th>
<th>$b_1$</th>
<th>$a_2$</th>
<th>$b_2$</th>
</tr>
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<tbody>
<tr>
<td>GaN</td>
<td>0.389</td>
<td>0.18</td>
<td>0.2</td>
<td>-0.44</td>
<td>0.67</td>
<td>-4.09</td>
<td>-8.87</td>
<td>-7.02</td>
<td>3.65</td>
</tr>
<tr>
<td>AlN</td>
<td>0.312</td>
<td>0.25</td>
<td>0.33</td>
<td>-0.53</td>
<td>1.50</td>
<td>-3.39</td>
<td>-11.81</td>
<td>-9.42</td>
<td>4.02</td>
</tr>
</tbody>
</table>

*Reference [14], †Reference [28], and ‡Reference [18].

Table 2: Band gap $E_g$ (in units of eV), spontaneous polarization (in units of C/m²), elastic constants $C_{11}$, $C_{12}$, $C_{13}$, and $C_{33}$ (in units of GPa), Phillips ionicity parameter $f_{ion}$, and the high frequency dielectric constant $\varepsilon_{\infty}$ for GaN and AlN.

<table>
<thead>
<tr>
<th></th>
<th>$E_g$</th>
<th>$P^s$</th>
<th>$C_{11}$</th>
<th>$C_{12}$</th>
<th>$C_{13}$</th>
<th>$C_{33}$</th>
<th>$f_{ion}$</th>
<th>$\varepsilon_{\infty}$</th>
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</thead>
<tbody>
<tr>
<td>GaN</td>
<td>3.507</td>
<td>-0.034</td>
<td>365</td>
<td>139</td>
<td>101</td>
<td>405</td>
<td>0.5</td>
<td>5.20</td>
</tr>
<tr>
<td>AlN</td>
<td>6.230</td>
<td>-0.090</td>
<td>397</td>
<td>143</td>
<td>112</td>
<td>371</td>
<td>0.499</td>
<td>4.30</td>
</tr>
</tbody>
</table>

*Reference [7], †Reference [28].

![Figure 3](image_url)  
**Figure 3:** The built-in electric field $F_{\text{GaN}}$ ($F_{\text{AlGaN}}$) in the well (barrier) layer along the QD growth direction as a function of the barrier thickness $L_b$ in WZ GaN/Al$_{1-x}$N strained QD with the QD thickness $L_w = 3$ nm, $P = 0$ GPa for different Al compositions $x$.

Can be given as follows. When Al composition $x$ increases, the equilibrium lattice constant $a_{eq}$ of the strained layer decreases according to (II); therefore, the absolute values of strain tensor $\varepsilon_{xx,b}$ and $\varepsilon_{zz,b}$ of the barrier layer along the QD growth direction increase, which induces that the piezoelectric polarization in the barrier layer increases, and then the BEF $F_{\text{GaN}}$ ($F_{\text{AlGaN}}$) increases correspondingly in (4).

In Figure 4, the ground-state donor binding energy is shown as a function of the QD radius in WZ GaN/Al$_{1-x}$N QD with the parameters ($L_w = 2$ nm, $L_b = 5$ nm, and $x = 0.3$) for different hydrostatic pressures ($P = 0$ Gpa, 4 Gpa, and 8 Gpa). The impurity ion is placed at the center of the QD. As shown in Figure 4, the donor binding energy increases with decreasing the radius $R$ in all cases, reaches a maximum value, and then decreases rapidly. The behavior is related to the variation of the electron confinement in QD; the electron wave function is firmly localized inside the QD with decreasing the QD radius. Therefore, the Coulomb interaction between the electron and the impurity ion is enhanced, and the donor binding energy increases correspondingly. Moreover, when the radial thickness decreases continuously to a certain value, the kinetic energy of the confined electron rises greatly, which increases greatly the probability of the electron penetrating into the potential barrier by the uncertainty principle and therefore the donor binding energy starts decreasing quickly. Moreover, Figure 4 also displays that the larger the hydrostatic pressure is, the bigger the donor binding energy is. The main reasons can be given as follows. With the increase of the hydrostatic pressure, the dielectric constants, the electron effective mass, and the finite confinement potential barrier will increase, which will result in bigger donor binding energy.

Figure 5 demonstrates that the ground-state donor binding energy in cylindrical WZ GaN/Al$_{1-x}$N strained QD as a function of the height $L_w$ with the parameters ($R = 10$ nm, $L_b = 20$ nm, and $x = 0.3$) for different hydrostatic pressures ($P = 0$ Gpa, 4 Gpa, and 8 Gpa). The impurity ion is placed at the center of the QD, setting $r_0 = 0$ and $z_0 = 0$. As expected, in all cases of hydrostatic pressures, the donor binding energy increases with a decrease of the QD height, reaches a maximum value, and then decreases quickly in finite potential barrier. For a fixed value of the barrier thickness $L_b$, the size quantization confinement of the electron wave function goes stronger with the decrease of the QD height, the electron-impurity Coulomb interaction becomes larger, and when the QD height becomes small enough, the probability of the electron leaking into the potential barrier increases greatly by the uncertainty principle. Therefore, the donor binding energy decreases correspondingly. In addition, the curves in Figure 5 also show that the stronger the applied hydrostatic pressure is, the bigger the donor binding energy is. Take the QD height $L_w = 4$ nm for example; a change of the hydrostatic pressure from 0 to 8 Gpa results in an increase of the impurity binding energy $E_{b}$ from 34.03 meV to 48.35 meV. As expected, with the increase of the hydrostatic pressure, the electron wave function is more localized, and then the donor binding energy decreases correspondingly.
Table 3: Strain coefficients of the zone-center phonon modes $K_{j,\zeta,xx}^r$ and $K_{j,\zeta,zz}^r$ (in units of cm$^{-1}$) for GaN and AlN.

<table>
<thead>
<tr>
<th></th>
<th>$K_{0,1,xx}$</th>
<th>$K_{0,1,zz}$</th>
<th>$K_{1,0,xx}$</th>
<th>$K_{1,0,zz}$</th>
<th>$K_{0,1,xx}$</th>
<th>$K_{0,1,zz}$</th>
<th>$K_{1,0,xx}$</th>
<th>$K_{1,0,zz}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaN</td>
<td>$-1139^a$</td>
<td>$-931^a$</td>
<td>$-300^a$</td>
<td>$-443^a$</td>
<td>$-1198^a$</td>
<td>$-885^a$</td>
<td>$-389^a$</td>
<td>$-618^a$</td>
</tr>
<tr>
<td>AlN</td>
<td>$-1208^a$</td>
<td>$-1330^a$</td>
<td>$-391^a$</td>
<td>$-70^a$</td>
<td>$-1233^a$</td>
<td>$-1038^a$</td>
<td>$-442^a$</td>
<td>$-434^a$</td>
</tr>
</tbody>
</table>

$^a$Reference [14].

Table 4: Band gap pressure coefficient $\chi$ (meV/GPa), phonon frequencies $\omega_{LO}$ and $\omega_{TO}$ (cm$^{-1}$) for GaN and AlN, and Gr"uneisen parameter of phonon mode $\gamma_{j,\zeta}$.

<table>
<thead>
<tr>
<th></th>
<th>$\chi$</th>
<th>$\omega_{TO}$</th>
<th>$\omega_{LO}$</th>
<th>$\omega_{TO}$</th>
<th>$\omega_{LO}$</th>
<th>$\gamma_{TO}$</th>
<th>$\gamma_{LO}$</th>
<th>$\gamma_{TO}$</th>
<th>$\gamma_{LO}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaN</td>
<td>$39^a$</td>
<td>$757^b$</td>
<td>$748^b$</td>
<td>$568^b$</td>
<td>$540^b$</td>
<td>$0.91^b$</td>
<td>$0.82^b$</td>
<td>$1.18^b$</td>
<td>$1.02^b$</td>
</tr>
<tr>
<td>AlN</td>
<td>$40^a$</td>
<td>$924^b$</td>
<td>$898^b$</td>
<td>$677^b$</td>
<td>$318^b$</td>
<td>$0.99^b$</td>
<td>$0.98^b$</td>
<td>$1.19^b$</td>
<td>$1.21^b$</td>
</tr>
</tbody>
</table>

$^a$Reference [29]; $^b$Reference [28].

**Figure 4:** The ground-state donor binding energy in cylindrical WZ GaN/Al$_{1-x}$Ga$_x$N strained QD as a function of the radius $R$ for $L_w = 2$ nm, $L_b = 5$ nm, $x = 0.3$ and several values of the hydrostatic pressure $P$.

**Figure 5:** The ground-state donor binding energy in cylindrical WZ GaN/Al$_{1-x}$Ga$_x$N strained QD as a function of the QD height ($L_w$) for $R = 10$ nm, $L_b = 20$ nm, $x = 0.3$ and several values of the hydrostatic pressure $P$.

The ground-state donor binding energy as a function of Al composition $x$ in WZ GaN/Al$_{1-x}$Ga$_x$N QD is displayed in Figure 6 for different hydrostatic pressures $P$. Numerical results show that the donor binding energy for the central impurity in WZ GaN/Al$_{1-x}$Ga$_x$N strained QD increases with the increase of Al composition. This is because that the competition effects between the built-in electric field and the potential barrier confinement will change the strength of the electron-impurity interaction. For the small QD height $L_w = 2$ nm, as the Al concentration increases, conductor band offset of WZ GaN/Al$_{1-x}$Ga$_x$N QD increases, and the potential barriers on the surfaces of QD play the main role in the distribution of the electron wave function. In addition, the bigger the Al composition $x$ is, the larger the potential barrier is, which results in the fact that the probability of the electron leaking into the barrier region becomes small. Accordingly, increasing the Coulomb effect between the electron and the impurity ion leads to the enhancement of the binding energy. Figure 6 also shows that the donor binding energy increases with the increment of the hydrostatic pressure $P$. This is due to the fact that the electron wave function is strongly compressed in the QD as hydrostatic pressure $P$ increases, and the strength of the electron-impurity interaction becomes larger, leading to the enhancement of the binding energy correspondingly.

To clarify the effect of the hydrostatic pressure on the ground-state donor binding energy, we investigated the...
Figure 6: The ground-state donor binding energy in cylindrical WZ GaN/Al$_{x}$Ga$_{1-x}$N strained QD as a function of Al composition $x$ for $R = 6$ nm, $L_w = 2$ nm, $L_b = 5$ nm, and several values of the hydrostatic pressure $P$.

Figure 7: The ground-state donor binding energy in cylindrical WZ GaN/Al$_{x}$Ga$_{1-x}$N strained QD as a function of the hydrostatic pressure ($P$) with $R = 5$ nm and $x = 0.1(0.3)$ and for different QD heights and barrier thicknesses.

Figure 8: The ground-state donor binding energy in cylindrical WZ GaN/Al$_{x}$Ga$_{1-x}$N strained QD as a function of the barrier thickness $L_b$ along the QD growth direction for $R = 10$ nm, $L_w = 3$ nm, $x = 0.2$ and several values of the hydrostatic pressure $P$.

The donor binding energy in cylindrical WZ GaN/Al$_{x}$Ga$_{1-x}$N strained QD with the parameters ($R = 5$ nm, $x = 0.1(0.3)$, $\rho_0 = 0$ nm, and $z_0 = 0$ nm) for several values of QD height and barrier thickness. From Figure 7, one can observe that the donor binding energy increases almost linearly as the hydrostatic pressure $P$ increases. The pressure behavior in WZ GaN/Al$_x$Ga$_{1-x}$N QD can be explained by the modification of the polarization in the dot layer by the pressure induced strain, which leads to a significant increase of the BEF $F_{\text{BEF}}$ in the QD. This behavior is in agreement with the result of [13]. In addition, the stronger the applied hydrostatic pressures is, the bigger the electron effective masses and dielectric constants of GaN and Al$_x$Ga$_{1-x}$N materials are, and the finite confinement potential at the boundary of GaN QD also becomes large under the bigger hydrostatic pressure; hence the expected value of the distance between the electron and the impurity ion reduces and the strength of the electron-impurity interaction becomes larger, which will lead to the increase of the donor binding energy correspondingly. Taking the solid curve for example, the donor binding energy increases by 21.15 meV approximately if the hydrostatic pressure $P$ increases from 0 to 8 GPa. Thus, the hydrostatic pressure has an important influence on the donor binding energy.

Figure 8 displays the ground-state donor binding energy as a function of the barrier thickness $L_b$ along the QD growth direction with the parameters ($R = 10$ nm, $L_w = 3$ nm, $\rho_0 = 0$ nm, $x = 0.2$ and $z_0 = 0$ nm) and different values of the hydrostatic pressure $P$. The impurity ion is located at the centre of the QD. We can see from Figure 8 that the donor binding energy increases, reaching a maximum value, and then reduces gradually with the increase of the barrier thickness $L_b$ in all cases. As expected, the curves in Figure 8 also show that the donor binding energy has a maximum value. This is because the enhancement of the barrier thickness leads to the change of the finite confinement potential along the QD growth direction. As the barrier thickness $L_b$ increases, the finite confinement potential at the bottom of the QD becomes small, and the one at the top of the QD becomes big due to the strong built-in electric field.
effects. When the QD barrier thickness $L_b$ increases to about 11 nm, the finite confinement potentials at two sides of the QD along the growth direction are approximately equal, which leads to the fact that the electron wave function is strongly compressed around the central impurity ion. Therefore, the Coulomb action between the electron and the impurity ion reaches a maximum.

In Figure 9, the ground-state donor binding energy is investigated as a function of the impurity position $z_0$ along the QD growth direction with the parameters ($R = 6$ nm, $L_w = 3$ nm, $L_b = 5$ nm, $x = 0.3$) and several values of the hydrostatic pressure $P$.

![Figure 9: The ground-state donor binding energy in a cylindrical WZ GaN/AlGaN strained QD as a function of the axial impurity position $z_0$ for $R = 6$ nm, $L_w = 3$ nm, $L_b = 5$ nm, $x = 0.3$ and several values of the hydrostatic pressure $P$.](image)

5. Conclusions

With the framework of the effective mass approximation, the ground-state donor binding energy in a cylindrical WZ GaN/Al$_x$Ga$_{1-x}$N strained QD is investigated theoretically in the presence of built-in electric field and hydrostatic pressure by using a variational approach. The ground-state donor binding energy depends strongly on dot radius, hydrostatic pressure, impurity position, and barrier thickness in the finite confinement potential. Numerical results show that the donor binding energy increases firstly, reaches a maximum value, and then drops slowly as the QD radius (height) decreases. And the donor binding energy is an increasing function of Al composition $x$ and/or hydrostatic pressure. In addition, the donor binding energy has a maximum value, when the impurity position moves along the symmetry axis of the QD from the bottom of the QD to the top, and the position of the peak value of the donor binding energy is also shifted towards positive $z$-direction. Moreover, the stronger the hydrostatic pressure is, the larger the peak value of the donor binding energy is with the same spatial confinement. The electronic wave function distribution in the QD is also obviously modified by the hydrostatic pressure. We hope that our results would stimulate further researches and lead to some potential applications on group-III nitride materials.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

Acknowledgments

This work was supported by the Scientific and Technological Department Foundation of Hebei Province (no. 12210617) and the Natural Science Foundation of Hebei Province (no. A201420308).

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