Research Article

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

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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_xGa_{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/AlGa_xN 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_xGa_{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/AlGa_xN strained QD, we calculate the donor binding energy of hydrogenic impurity in a WZ GaN/AlGa_xN 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_xGa_{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_xGa_{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_xGa_{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_xGa_{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_xGa_{1-x}N QD under the influence of hydrostatic pressure can be written [4] as

$$\hat{H} = \hat{H}_0 - \frac{e^2}{4\pi\epsilon_0\bar{\epsilon}(p)|\vec{r} - \vec{r}_0|}, \quad (1)$$

where $\vec{r}(\vec{r}_0)$ denotes the position vector of the electron (impurity ion), e is the absolute value of the electron charge, ϵ_0 is the permittivity of free space, and $\bar{\epsilon}(p)$ is the pressure-dependent effective mean relative dielectric constant of GaN and Al_xGa_{1-x}N materials. The Hamiltonian $\hat{H}_0$ is given by [11]

$$\begin{aligned} \hat{H}_0 = & -\frac{\hbar^2}{2m_{\perp}(p)} \left(\frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2}{\partial \varphi^2} \right) \\ & - \frac{\hbar^2}{2m_{\parallel}(p)} \frac{\partial^2}{\partial z^2} + V(\rho, z, p) - eF_{w,b}(p)z, \end{aligned} \quad (2)$$

where $m_{\parallel}$ and $m_{\perp}$ are the pressure- and strain-dependent effective masses of electron along and perpendicular to the

[0001]-direction. And $V(\rho, z, p)$ is the electron confinement potential due to the band offset ($Q_j = 0.765$) and is given by [13]

$$V(z, p) = \begin{cases} Q_j [E_{g, \text{Al}_x\text{Ga}_{1-x}\text{N}} - E_{g, \text{GaN}}], & \frac{L_w}{2} < z < \frac{L_w}{2} + \frac{L_b}{2}, \\ -\frac{L_w}{2} - \frac{L_b}{2} < z < -\frac{L_w}{2}, \\ 0 & |z| \leq \frac{L_w}{2}, \end{cases} \quad (3)$$

$$V(\rho, p) = \begin{cases} 0, & \rho \leq R, \\ Q_j [E_{g, \text{Al}_x\text{Ga}_{1-x}\text{N}} - E_{g, \text{GaN}}] & \text{others.} \end{cases} \quad (4)$$

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

$$F_{\text{GaN}}(p) = \left| \frac{L_b (P_{\text{sp}}^{\text{AlGa}} + P_{\text{pe}}^{\text{AlGa}} - P_{\text{sp}}^{\text{GaN}} - P_{\text{pe}}^{\text{GaN}})}{\epsilon_0 (L_b \epsilon_e^{\text{GaN}} + L_w \epsilon_e^{\text{AlGa}})} \right|, \quad (5)$$

$$F_{\text{AlGa}}(p) = -\frac{L_w}{L_b} F_{\text{GaN}}(p),$$

where L_w , L_b and ϵ_e^{GaN} , ϵ_e^{AlGa} are the thicknesses and electronic dielectric constants for GaN and Al_xGa_{1-x}N materials, $P_{\text{sp}}^{\text{GaN}}$, $P_{\text{sp}}^{\text{AlGa}}$ and $P_{\text{pe}}^{\text{GaN}}$, $P_{\text{pe}}^{\text{AlGa}}$ are the spontaneous and piezoelectric polarizations for GaN and Al_xGa_{1-x}N materials, and the bowing parameter η is chosen as -0.019 C/m^2 [14]:

$$P_{\text{sp}}^{\text{AlGa}} = xP_{\text{sp}}^{\text{AlN}} + (1-x)P_{\text{sp}}^{\text{GaN}} - \eta x(1-x). \quad (6)$$

The wave function of the electron confined in the WZ GaN/Al_xGa_{1-x}N QD can be written as

$$\begin{aligned} \psi(\rho, \varphi, z) &= f(\rho) h(z) e^{im\varphi}, \quad m = 0, \pm 1, \pm 2, \dots, \\ f(\rho) &= \begin{cases} J_0(\beta\rho) & \rho \leq R, \\ \frac{J_0(\beta R)}{K_0(\beta R)} K_0(\alpha\rho) & \rho > R, \end{cases} \end{aligned} \quad (7)$$

where the constants (α and β) 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 J_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]:

$$h(z) = \begin{cases} C_1 \text{Ai}(\varepsilon_1) + D_1 \text{Bi}(\varepsilon_1) & -\frac{L_w}{2} - L_b < z < -\frac{L_w}{2}, \\ C_2 \text{Ai}(\varepsilon_2) + D_2 \text{Bi}(\varepsilon_2) & |z| \leq \frac{L_w}{2}, \\ C_3 \text{Ai}(\varepsilon_3) + D_3 \text{Bi}(\varepsilon_3) & \frac{L_w}{2} < z < \frac{L_w}{2} + L_b. \end{cases} \quad (8)$$

Here $\varepsilon_j = ((2m_j^*/\hbar^2)eF)^{1/3}(z - E_z - V(z, p)/eF)$. The coefficients C_j and D_j ($j = 1, 2$, and 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]

$$\phi(\rho, \varphi, z) = N\psi(\rho, \varphi, z)e^{-\alpha(\rho-\rho_0)^2-\beta(z-z_0)^2}, \quad (9)$$

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,

$$E_b = E_{0\rho} + E_{0z} - \min_{\alpha, \beta} \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}. \quad (10)$$

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 AlGaIn materials are given under the hydrostatic pressure P [18]:

$$\begin{aligned} \varepsilon_{xx, \text{GaN}} = \varepsilon_{yy, \text{GaN}} &= \frac{a_{\text{eq}}(p) - a_{\text{GaN}}(P)}{a_{\text{GaN}}(P)}, \\ \varepsilon_{xx, \text{AlGaIn}} = \varepsilon_{yy, \text{AlGaIn}} &= \frac{a_{\text{eq}}(p) - a_{\text{AlGaIn}}(P)}{a_{\text{AlGaIn}}(P)}, \end{aligned} \quad (11)$$

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]:

$$a_{\text{eq}}(p) = \frac{a_{\text{GaN}}L_w + a_{\text{AlGaIn}}L_b}{L_w + L_b}. \quad (12)$$

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

$$a_\nu(P) = a_{0,\nu} \left(1 - \frac{P}{3B_{0,\nu}} \right), \quad \nu = \text{GaN, AlN}. \quad (13)$$

Here the actual lattice constant a_{AlGaIn} of the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ material can be obtained by the linear interpolation method from the corresponding values of GaN and AlN. $L_{\text{GaN}}(L_{\text{AlGaIn}})$ 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]

$$\begin{aligned} \varepsilon_{zz, \text{GaN}} &= R_{\text{GaN}}^H \varepsilon_{xx, \text{GaN}}, \\ \varepsilon_{zz, \text{AlGaIn}} &= R_{\text{AlGaIn}}^H \varepsilon_{xx, \text{AlGaIn}}. \end{aligned} \quad (14)$$

The coefficient R_ν^H of the GaN (AlN) material is given by [21]

$$R_\nu^H = \frac{C_{11,\nu}(P) + C_{12,\nu}(P) - 2C_{13,\nu}(P)}{C_{33,\nu}(P) - C_{13,\nu}(P)}, \quad \nu = \text{GaN, AlN}, \quad (15)$$

where $C_{\lambda\kappa,\nu}$ is the pressure-dependent elastic stiffness constant of material ν and is given by [21] $C_{\lambda\kappa,\nu}(P) = C_{\lambda\kappa,\nu}(0) + \sigma_{\lambda\kappa,\nu}P + \delta_{\lambda\kappa,\nu}P^2$ and the coefficient R_{AlGaIn}^H and the pressure-dependent elastic stiffness constant $C_{\lambda\kappa, \text{AlGaIn}}$ of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ 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]

$$\begin{aligned} E_{g, \text{GaN}} &= E_{g, \text{GaN}}(p) + 2(a_{1, \text{GaN}} + b_{1, \text{GaN}})\varepsilon_{xx, \text{GaN}} \\ &\quad + (a_{2, \text{GaN}} + b_{2, \text{GaN}})\varepsilon_{zz, \text{GaN}}, \end{aligned} \quad (16)$$

$$E_{g, \text{AlN}} = E_{g, \text{AlN}}(p) + 2a_{1, \text{AlN}}\varepsilon_{xx, \text{AlN}} + a_{2, \text{AlN}}\varepsilon_{zz, \text{AlN}},$$

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]:

$$E_{g,\nu}(p) = E_{g,\nu}(0) + \chi_\nu p. \quad (17)$$

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

$$E_{g, \text{AlGaIn}}(p) = (1-x)E_{g, \text{GaN}} + xE_{g, \text{AlN}} - bx(1-x). \quad (18)$$

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]

$$\frac{m_0}{m_\nu^{\perp, //}(p)} = 1 + \frac{C_{j,\nu}}{E_{g,\nu}(p)}, \quad (19)$$

where $C_{j,\nu}$ is a fixed value for a given material ν and can be derived from the values of $m_\nu^{\perp, //}(0)$ 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 ε_ξ is influenced by biaxial strain and hydrostatic pressure. The tensor components of ε_ξ^ν for the WZ structure are derived from the generalized Lyddane-Sachs-Teller relation [24]:

$$\varepsilon_\xi^\nu(p) = \varepsilon_{\infty, \xi}^\nu(p) \left(\frac{\omega_{\text{LO}, \xi}^\nu(p)}{\omega_{\text{TO}, \xi}^\nu(p)} \right)^2, \quad (20)$$

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

$$\omega_{j,\xi}^\nu = \omega_{j,\xi}^\nu(p) + 2K_{j,\xi,xx}^\nu \varepsilon_{xx,\nu}(p) + K_{j,\xi,zz}^\nu \varepsilon_{zz,\nu}(p). \quad (21)$$

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

$$\gamma_{j,\xi}^\nu = B_{0,\nu} \frac{1}{\omega_{j,\xi}^\nu(0)} \left(\frac{\partial \omega_{j,\xi}^\nu(p)}{\partial p} \right), \quad (22)$$

where the subscript j represents LO or TO phonon, ξ ($\xi = \perp$ or z) denotes x - y plane or z -direction, $\omega_{j,\xi}^\nu(0)$ is the zone-center phonon frequency of material ν , $\gamma_{j,\xi}^\nu$ is Grüneisen parameter of phonon mode given in [25], $B_{0,\nu}$ is bulk modulus, and $K_{j,\xi,xx}^\nu$ and $K_{j,\xi,zz}^\nu$ are the strain coefficients of zone-center phonon modes. Following [14], the influence of hydrostatic pressure on the high frequency dielectric constants can be written as

$$\frac{\partial \varepsilon_{\infty,\xi}^\nu(p)}{\partial p} = -\frac{5(\varepsilon_{\infty,\xi}^\nu - 1)}{3B_{0,\nu}} (0.9 - f_{\text{ion}}^\nu). \quad (23)$$

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

$$B_{0,\nu} = \frac{(C_{11,\nu}(P) + C_{12,\nu}(P))C_{33,\nu}(P) - 2C_{13,\nu}^2(P)}{C_{11,\nu}(P) + C_{12,\nu}(P) + 2C_{33,\nu}(P) - 4C_{13,\nu}(P)}, \quad (24)$$

where $C_{11,\nu}$, $C_{12,\nu}$, $C_{13,\nu}$, and $C_{33,\nu}$ are the elastic constants of material ν . The effective mean relative dielectric constant in (1) is defined as [26]

$$\bar{\varepsilon}_\nu(p) = \frac{2}{3}\varepsilon_{\xi,\perp}^\nu(p) + \frac{1}{3}\varepsilon_{\xi,z}^\nu(p). \quad (25)$$

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

$$P_{\text{pe}}^\nu = e_{33}^\nu(p) \varepsilon_{zz}^\nu + 2e_{31}^\nu(p) \varepsilon_{xx}^\nu, \quad (26)$$

where e_{31}^ν and e_{33}^ν are the pressure-dependent piezoelectric constants of material ν .

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 $\text{GaN}/\text{Al}_x\text{Ga}_{1-x}\text{N}$ strained QD. All material parameters used in our calculations are listed in Tables 1–4. Material parameters of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ are estimated using a linear interpolation between the values of the corresponding parameters of GaN and AlN.

FIGURE 2: The built-in electric field F_{GaN} (F_{AlGaN}) in the well (barrier) layer along the QD growth direction as a function of the barrier thickness L_b in WZ $\text{GaN}/\text{Al}_x\text{Ga}_{1-x}\text{N}$ strained QD with the QD height $L_w = 3$ nm, $x = 0.3$ for different hydrostatic pressures P .

Figure 2 presents that the built-in electric field (BEF) F_{GaN} (F_{AlGaN}) in the well (barrier) layer along the growth direction z -axis as a function of the barrier thickness L_b in WZ $\text{GaN}/\text{Al}_x\text{Ga}_{1-x}\text{N}$ QD for different hydrostatic pressures P . Numerical results show that the BEF F_{GaN} (F_{AlGaN}) is an increasing (a decreasing) function of the barrier thickness L_b . This is because the fact that the equilibrium lattice constant a_{eq} of the strained layer and the components of the strain tensor $\varepsilon_{xx,w}$ of the dot layer decrease with the increase of the barrier thickness L_b according to (11), which induces the decrement of the piezoelectric polarization in the dot layer and the increment of the piezoelectric polarization in the barrier layer along the QD growth direction. Therefore, the BEF F_{GaN} (F_{AlGaN}) gradually increases (decreases) (see (5)). Moreover, Figure 2 also shows that the built-in electric fields (F_{GaN} and F_{AlGaN}) increase correspondingly as the hydrostatic pressure P increases; this is caused by the change of the pressure-dependent piezoelectric constants, the biaxial strains, and the dielectric constants of WZ $\text{GaN}/\text{Al}_x\text{Ga}_{1-x}\text{N}$ QD when the hydrostatic pressure increases.

In Figure 3, the built-in electric field (BEF) F_{GaN} (F_{AlGaN}) in the well (barrier) layer along the QD growth direction z -axis is displayed as a function of the barrier thickness L_b for different Al compositions x in WZ $\text{GaN}/\text{Al}_x\text{Ga}_{1-x}\text{N}$ QD. Numerical results show that the BEF F_{GaN} (F_{AlGaN}) increases (decreases) gradually when the barrier thickness L_b increases. This is caused by the change of the pressure-dependent piezoelectric constants, the biaxial strains, and the dielectric constants of WZ $\text{GaN}/\text{Al}_x\text{Ga}_{1-x}\text{N}$ strained QD. In addition, Figure 3 also shows that the BEF F_{GaN} (F_{AlGaN}) increases as Al composition x increases, but the BEF F_{AlGaN} remains insensitive to the bigger barrier thickness L_b . The reason

TABLE 1: Lattice constant a (in units of nm), effective mass m_e (in units of a free-electron mass m_0), piezoelectric constants e_{31} and e_{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.

	a	$m_{\perp}$	$m_{\parallel}$	e_{31}	e_{33}	a_1	b_1	a_2	b_2
GaN	0.3189 ^a	0.18 ^a	0.2 ^a	-0.44 ^b	0.67 ^b	-4.09 ^c	-8.87 ^c	-7.02 ^c	3.65 ^c
AlN	0.3112 ^a	0.25 ^a	0.33 ^a	-0.53 ^b	1.50 ^b	-3.39 ^c	-11.81 ^c	-9.42 ^c	4.02 ^c

^aReference [14], ^bReference [28], and ^cReference [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 ϵ_{∞} for GaN and AlN.

	E_g	p^{sp}	C_{11}	C_{12}	C_{13}	C_{33}	f_{ion}	$\epsilon_{\infty,\perp}$	$\epsilon_{\infty,z}$
GaN	3.507 ^a	-0.034 ^a	365 ^b	139 ^b	101 ^b	405 ^b	0.5 ^a	5.20 ^a	5.39 ^a
AlN	6.230 ^a	-0.090 ^a	397 ^b	143 ^b	112 ^b	371 ^b	0.499 ^a	4.30 ^a	4.52 ^a

^aReference [7]; ^bReference [28].

FIGURE 3: The built-in electric field F_{GaN} (F_{AlGaN}) in the well (barrier) layer along the QD growth direction as a function of the barrier thickness L_b in WZ GaN/Al_xGa_{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 (11); therefore, the absolute values of strain tensor $\epsilon_{xx,b}$ and $\epsilon_{zz,b}$ 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_{GaN} (F_{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_xGa_{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_xGa_{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 $\rho_0 = 0$ 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

TABLE 3: Strain coefficients of the zone-center phonon modes $K_{j,\xi,xx}^\nu$ and $K_{j,\xi,zz}^\nu$ (in units of cm^{-1}) for GaN and AlN.

	$K_{\text{TO},\perp,xx}^\nu$	$K_{\text{TO},\parallel,xx}^\nu$	$K_{\text{TO},\perp,zz}^\nu$	$K_{\text{TO},\parallel,zz}^\nu$	$K_{\text{LO},\perp,xx}^\nu$	$K_{\text{LO},\parallel,xx}^\nu$	$K_{\text{LO},\perp,zz}^\nu$	$K_{\text{LO},\parallel,zz}^\nu$
GaN	-1139 ^a	-931 ^a	-300 ^a	-443 ^a	-1198 ^a	-885 ^a	-389 ^a	-618 ^a
AlN	-1208 ^a	-1330 ^a	-391 ^a	-70 ^a	-1233 ^a	-1038 ^a	-442 ^a	-434 ^a

^aReference [14].TABLE 4: Band gap pressure coefficient χ (meV/GPa), phonon frequencies ω_{LO} and ω_{TO} (cm^{-1}) for GaN and AlN, and Grüneisen parameter of phonon mode $\gamma_{j,\xi}^\nu$.

	χ	$\omega_{\text{LO},\perp}$	$\omega_{\text{LO},\parallel}$	$\omega_{\text{TO},\perp}$	$\omega_{\text{TO},\parallel}$	$\gamma_{\text{LO},\perp}$	$\gamma_{\text{LO},\parallel}$	$\gamma_{\text{TO},\perp}$	$\gamma_{\text{TO},\parallel}$
GaN	39 ^a	757 ^b	748 ^b	568 ^b	540 ^b	0.91 ^b	0.82 ^b	1.18 ^b	1.02 ^b
AlN	40 ^a	924 ^b	898 ^b	677 ^b	318 ^b	0.99 ^b	0.98 ^b	1.19 ^b	1.21 ^b

^aReference [29]; ^bReference [28]. FIGURE 4: The ground-state donor binding energy in cylindrical WZ GaN/Al_xGa_{1-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_xGa_{1-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 .

pressure p , electron effective masses and dielectric constants of GaN and Al_xGa_{1-x}N materials become larger, and a growth of the hydrostatic pressure leads to the increase of the finite potential barrier, which will lead to the electron wave function being firmly squeezed around the impurity ion, and consequently the donor binding energy increases correspondingly.

The ground-state donor binding energy as a function of Al composition x in WZ GaN/Al_xGa_{1-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_xGa_{1-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_xGa_{1-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_xGa_{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_xGa_{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.

donor binding energy in cylindrical WZ GaN/Al_xGa_{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_xGa_{1-x}N QD can be explained by

FIGURE 8: The ground-state donor binding energy in cylindrical WZ GaN/Al_xGa_{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 modification of the polarization in the dot layer by the pressure induced strain, which leads to a significant increase of the BEF F_{GaN} 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_xGa_{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

FIGURE 9: The ground-state donor binding energy in a cylindrical WZ GaN/Al_xGa_{1-x}N 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 .

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, $x = 0.3$ and $\rho_0 = 0$ nm) and different values of the hydrostatic pressure P . As shown in Figure 9 the curves in all cases are absolutely asymmetry, and the donor binding energy demonstrates a maximum value when the impurity is located from the plane $z = -L_w/2$ to the symmetry plane $L_w/2$ along the growth direction of the QD, and the maximum value of the donor binding energy is not located at the point $[0, 0]$. This is because the fact that the strong BEF modifies the spread of the electron wave function in the QD, and the direction of the built-in electric field F_w in the dot layer is opposite to the growth direction of the QD. Thus, the built-in electric field F_w pushes the electron toward the right side of the QD. This behavior is in agreement with the result of [17]. In addition, the curves also show that the stronger the hydrostatic pressure is, the larger the peak value of the donor binding energy is with the same parameters (L_w , R , and ρ_0). Moreover, the position of the peak value of the donor binding energy is also shifted to positive z -direction. This is because the fact that the electronic wave function is obviously modified, and the bigger concentration of the electron wave function is squeezed strongly around the impurity ion. In addition, the stronger the hydrostatic pressure is, the bigger

the localization effect of the electron wave function is, so that the peak value of the binding energy increases accordingly. Therefore, the distribution of the electron wave function is not central symmetrical about the QD in the presence of the strong BEF.

5. Conclusions

With the framework of the effective mass approximation, the ground-state donor binding energy in a cylindrical WZ GaN/Al_xGa_{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.

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