Correlated electron–hole transitions in wurtzite GaN quantum dots: the effects of strain and hydrostatic pressure*

Zheng Dongmei(郑冬梅)†, Wang Zongchi(王宗箴), and Xiao Boqi(肖波齐)

Department of Physics and Electromechanical Engineering, Sanming College, Sanming 365004, China

Abstract: Within the effective-mass and finite-height potential barrier approximation, a theoretical study of the effects of strain and hydrostatic pressure on the exciton emission wavelength and electron–hole recombination rate in wurtzite cylindrical GaN/AlGaN quantum dots (QDs) is performed using a variational approach. Numerical results show that the emission wavelength with strain effect is higher than that without strain effect when the QD height is large (> 3.8 nm), but the status is opposite when the QD height is small (< 3.8 nm). The height of GaN QDs must be less than 5.5 nm for an efficient electron–hole recombination process due to the strain effect. The emission wavelength decreases linearly and the electron–hole recombination rate increases almost linearly with applied hydrostatic pressure. The hydrostatic pressure has a remarkable influence on the emission wavelength for large QDs, and has a significant influence on the electron–hole recombination rate for small QDs. Furthermore, the present numerical outcomes are in qualitative agreement with previous experimental findings under zero pressure.

Key words: GaN quantum dots; excitons; strain; hydrostatic pressure
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1. Introduction

Wide band-gap wurtzite III–V nitrides have been widely used in recent years in the design and fabrication of optical devices such as high-brightness blue/green light emitting diodes (LEDs)[1,2] and laser diodes[3,4]. Recently, it was found that the electronic and optical properties of wurtzite (WZ) GaN/AlGaN quantum heterostructures are affected by the built-in electric field (BEF) induced by the piezoelectricity and spontaneous polarizations. The magnitude of the BEF was estimated to be in the order of MV/cm[5,6]. The exciton states and optical properties of strained GaN/AlGaN heterostructures have been investigated[7–13]. These studies showed that a strong BEF leads to a remarkable reduction in the effective band-gap of the heterostructures and gives a significant spatial separation of the electrons and holes in the WZ GaN/AlGaN quantum heterostructures. However, none of these calculations included the strain dependence of the material parameters.

The hydrostatic pressure modifications of the physical properties of nitride-based low-dimensional structures are available and helpful for exploring new phenomena and improving devices[12,13]. Wagner et al.[14] presented *ab initio* calculations of the structural, dielectric and lattice-dynamical properties of GaN and AlN under hydrostatic pressure. Goji et al.[15] investigated, experimentally, the pressure modification of the phonon modes in wurtzite and zinc-blende GaN and wurtzite AlN. Lpkowski et al.[16] studied the influence of hydrostatic pressure on the light emission from a strained GaN/AlGaN multi-quantum-well system. It was found that the coefficient describing the pressure dependence of the photoluminescence peak energy was reduced with respect to the pressure dependence of the energy gap. This could be explained by the hydrostatic pressure-induced increase in the piezoelectric field in the quantum structures. Ha et al.[17] explored the influences of screening and hydrostatic pressure on the binding energies of heavy-hole excitons in a strained wurtzite GaN/Al0.3Ga0.7N quantum well and obtained two important conclusions: (1) the binding energies of excitons increased almost linearly with pressure, and (2) the exciton binding energies increased obviously with decreasing barrier thickness due to the built-in electric field. To our knowledge, calculations of the interband optical transitions due to the excitons influenced by hydrostatic pressure in wurtzite GaN/Al0.3Ga0.7N cylindrical quantum dots (QDs) considering the strong BEF effect and strain dependence of material parameters, are still absent at present. In this paper we study, variationally, the effects of strain (including the strong BEF and the strain dependence of material parameters) and hydrostatic pressure on the interband optical transition and electron–hole recombination rate of heavy-hole excitons confined in a wurtzite GaN/Al0.3Ga0.7N cylindrical QD with finite height potential barriers.

2. Theoretical model

2.1. Variational calculation of the exciton states

Let us now consider an isolated cylindrical GaN QD with radius $R$ and height $L$ surrounded by a large energy gap material $Al_{1-x}Ga_{x}N$, in which the origin is taken at the center of the QD and the $z$ axis is defined to be the growth direction (see Fig. 1). Within the framework of effective mass, the Hamilto-
Fig. 1. A diagram of a wurtzite GaN cylindrical QD with radius $R$ and height $L$ surrounded by the large energy-gap material wurtzite Al$_x$Ga$_{1-x}$N, in which the origin is taken at the center of the QD and the $z$ direction is defined to be the growth direction.

The Hamiltonian of the electron (hole) in the cylindrical coordinates reads

$$
\hat{H}_j = -\frac{\hbar^2}{2m_j^*} \left[ \frac{1}{\rho_j} \frac{\partial}{\partial \rho_j} \left( \rho_j \frac{\partial}{\partial \rho_j} \right) + \frac{1}{\rho_j^2} \frac{\partial^2}{\partial \varphi_j^2} + \frac{\partial^2}{\partial z_j^2} \right] + V(\rho_j) + V(z_j) + eEz_j,
$$

where $V(\rho_j)$ and $V(z_j)$ are the in-plane and $z$-direction confinement potential due to the band offset ($Q_j$) in the WZ GaN/Al$_x$Ga$_{1-x}$N QD, respectively. They can be given by

$$
V(\rho_j) = \begin{cases} 
0, & \rho_j \leq R, \\
Q_j \left[ E_g(Al_xGa_{1-x}N) - E_g(GaN) \right], & \rho_j > R.
\end{cases} 
$$

In this paper, the ratio of the conduction band to the valence band offset is assumed to be 75 : 25$^{[19]}$.

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

$$\psi_j(\rho_j, \varphi_j, z_j) = f(\rho_j)h(z_j)e^{im\varphi_j}, \quad m = 0, \pm 1, \pm 2, \ldots,$$

where $m$ is the electron (hole) $z$-component angular momentum number. The radial wave function $f(\rho_j)$ of the electron (hole) can be obtained using the Bessel function $J_m$ and the modified Bessel function $K_m$. Wave function $h(z_j)$ can be expressed by means of the Airy functions $A_l$ and $B_l$.

In order to calculate the exciton binding energy, the trial wave function can be chosen as$^{[10, 20-22]}$

$$\Phi_{ex}(r_e, r_h) = \psi_e(\rho_e, \varphi_e, z_e)\psi_h(\rho_h, \varphi_h, z_h)e^{-a\rho_e^2e^{-\beta z_e}},$$

where $\psi_e(\psi_h)$ is the electron (hole) wave function confined in the QD, $\rho_{eh}^2 = \rho_e^2 + \rho_h^2 - 2\rho_e\rho_h \cos(\varphi_e - \varphi_h)$, $z_{eh}^2 = (z_e - z_h)^2$, and $\alpha$ and $\beta$ are variational parameters.

The ground-state energy of the exciton can be determined by

$$E_{ex} = \min_{\alpha, \beta} \frac{|\Phi_{ex}|\hat{H}_{ex}|\Phi_{ex}|}{(|\Phi_{ex}|\hat{E}_{ex}|\Phi_{ex}|)^{1/2}}.$$

The exciton binding energy $E_b$ and the optical transition energy $E_{ph}$ can be defined as follows,

$$E_b = E_e + E_h - E_{ex},$$

$$E_{ph} = E_e + E_h + E_{ex} - E_b,$$

where $E_e$ is the effective band-gap energy of the GaN material, and $E_x$ ($E_h$) is the electron (hole) confinement energy in the QD.

The emission wavelength associated with the exciton can be represented as

$$\lambda = \frac{\hbar c}{E_e + E_{ex}}.$$

The probability of radiative transition associated with the exciton states described by the wave function (Eq. (7)) is proportional to the square of the overlap integral defined as$^{[26]}$

$$M_{ex-h}^2 = \int d\rho_e d\rho_h \Phi_{ex}(r_e, r_h)\delta(r_e - r_h)^2.$$

### 2.2. Pressure and strain dependence of the parameters

The pressure- and strain-dependent energy gaps of GaN and AlN are$^{[23]}$

$$E_{g,GaN} = E_{g,GaN}(P) + 2(a_{2,GaN} + b_{2,GaN})\varepsilon_{xx,GaN} + (a_{1,GaN} + b_{1,GaN})\varepsilon_{zz,GaN},$$

$$E_{g,AlN} = E_{g,AlN}(P) + 2a_{2,AlN}\varepsilon_{xx,AlN} + a_{1,AlN}\varepsilon_{zz,AlN}.$$
where \(a_{i;j} \), \(a_{j;i} \), \(b_{1;j} \) and \(b_{2;j} \) (\(i = \text{GaN} \) or \(\text{AlN} \)) are the deformation potentials. The dependence of the energy gap on hydrostatic pressure \(P\) is considered by the following equation\[17\]

\[
E_{g,i}(P) = E_{g,i}(0) + \chi_i P.
\] (15)

The energy gap of the ternary mixed crystal \(\text{Al}_x\text{Ga}_{1-x}\text{N} \) (chosen as the barriers) is\[19\]:

\[
E_{g,\text{Al}_x\text{Ga}_{1-x}\text{N}} = E_{g,\text{GaN}}(1 - x) + E_{g,\text{AlN}}x
- 1.3(\text{eV}) x(1 - x).
\] (16)

Within the infinitely thick barrier approximation, the biaxial lattice-mismatch induced strains in the GaN QD are given\[24\]:

\[
\varepsilon_{xx,\text{GaN}} = \varepsilon_{yy,\text{GaN}} = \frac{a_{\text{AlGaN}}(P) - a_{\text{GaN}}(P)}{a_{\text{GaN}}(P)}.
\] (17)

where \(a_{\text{AlGaN}}(P)\) and \(a_{\text{GaN}}(P)\) represent the \(a\)-axis lattice constant of \(\text{Al}_x\text{Ga}_{1-x}\text{N} \) and GaN. The lattice constant as a function of hydrostatic pressure is given by\[25\]:

\[
a_i(P) = a_{0i}(1 - \frac{P}{3B_{0i}}),
\] (18)

where superscript \(i = w \) or \(b \) donates the well or barrier materials. The bulk modulus \(B_{0i}\) in a wurtzite structure is given by elastic constants \(C_{11}, C_{12}, C_{13}\) and \(C_{33}\) as\[24\]:

\[
B_{0i} = \frac{(C_{11,i} + C_{12,i})C_{33,i} - 2C_{13,i}^2}{C_{11,i} + C_{12,i} + 2C_{33,i} - 4C_{13,i}}.
\] (19)

Based on the Hooke’s law, the ratio of the in-plane strain component and the strain component along the \(c\) axis can be expressed by\[24\]:

\[
\frac{\varepsilon_{zz,i}}{\varepsilon_{xx,i}} = \frac{C_{11,i} + C_{12,i} - 2C_{13,i}}{C_{33,i} - C_{13,i}}.
\] (20)

The strain and hydrostatic pressure dependences of the effective masses of an electron in the \(z\) direction and the \(x\)-\(y\) plane can be calculated by\[26\]:

\[
\frac{m_0}{m_{0e,i}^{1//2}}(P) = 1 + \frac{C}{E_{g,i}}.
\] (21)

Here, \(C\) is a constant and can be determined by solving Eq. (21) at \(P = 0\). In general, the pressure coefficient for a heavy-hole is assumed to be zero.

Static dielectric constant \(\varepsilon_s\) is influenced by the strain and hydrostatic pressure, respectively. The tensor components of \(\varepsilon_s\) for the wurtzite structure are derived from the generalized Lyddane–Sachs–Tellier relation\[24\]:

\[
\varepsilon_{s,\delta\delta} = \varepsilon_{\infty,\delta\delta} \left(\frac{\omega_{LO,\delta\delta}}{\omega_{TO,\delta\delta}}\right)^2.
\] (22)

The frequencies of LO and TO phonons influenced by pressure and strain in Eq. (22) can be written as\[24\]:

\[
\omega_{j,\delta\delta} = \omega_{j,\delta\delta}(P) + 2K_{j,xx}\varepsilon_{xx} + K_{j,zz}\varepsilon_{zz}'.
\] (23)

where \(K_{j,xx}\) and \(K_{j,zz}\) are the strain coefficients of the phonon modes given in Ref. [24], and \(j\) represents the LO or TO phonon. The tensor component \((\delta = z, x)\) is related to the LO and TO phonon frequencies, respectively. Furthermore, the hydrostatic pressure dependence of \(\omega_{j,\delta\delta}(P)\) can be determined by the given mode Grüneisen parameter\[27\]:

\[
\gamma_{j,\delta\delta} = B_0 \frac{1}{\omega_{j,\delta\delta}} \frac{\partial \omega_{j,\delta\delta}(P)}{\partial P}.
\] (24)

Considering the influence of hydrostatic pressure, the high-frequency dielectric constant in Eq. (22) can be written as\[28\]:

\[
\frac{\partial \varepsilon_{\infty,\delta\delta}(P)}{\partial P} = -\frac{5(\varepsilon_{\infty,\delta\delta} - 1)}{3B_0} (0.9 - f_{\text{ion}}),
\] (25)

where \(f_{\text{ion}}\) is the ionicity of the material under pressure.

The effective mean relative dielectric constant in Eq. (1) is defined as

\[
\bar{\varepsilon}(P) = \frac{2}{3} \varepsilon_{s,xx}(P) + \frac{1}{3} \varepsilon_{s,zz}(P).
\] (26)

The strain-induced piezoelectric polarization in Eq. (3) is written as\[29\]:

\[
P^{\text{pie}}_{31} = 2\varepsilon_{31}(P)\varepsilon_{s,xx} + \varepsilon_{33}(P)\varepsilon_{s,zz},
\] (27)

where \(\varepsilon_{31}\) and \(\varepsilon_{33}\) are the strain-dependent piezoelectric constants of GaN satisfying\[29\]:

\[
\varepsilon_{31}(P) = \varepsilon_{31}(0) + \frac{4Z^*e}{\sqrt{3}a_{\text{GaN}}(P)} \frac{d\mu}{dx_{xx}},
\] (28)

\[
\varepsilon_{33}(P) = \varepsilon_{33}(0) + \frac{4Z^*e}{\sqrt{3}a_{\text{GaN}}(P)} \frac{d\mu}{dx_{zz}},
\] (29)

where \(\varepsilon_{31}(0)\) and \(\varepsilon_{33}(0)\) are the clamped-ion terms that represent the effects of strain on the electronic structure, and the second term in Eqs. (28) and (29) is the contribution resulting from the relative displacement of the anion and cation sublattices (internal strain term). The other quantities in Eqs. (28) and (29) are the Born effective charge \(Z^*\) along the \(c\) axis, the lattice constant \(a_{\text{GaN}}(P)\) of GaN, and the internal parameter \(\mu\). From Ref. [24], we can obtain \(Z^* = 1.18, \frac{d\mu}{dx_{xx}} = -0.208, \frac{d\mu}{dx_{zz}} = 0.262\).

The pressure-dependent radius and height of the GaN QD may be obtained from the fractional change in volume associated with the hydrostatic pressure\[30\]:

\[
\frac{\Delta V}{V_0} = -3P(S_{11} + 2S_{12}),
\] (30)

with \(V(P) = \pi R^2(P)L(P), V_0 = \pi R_0^2L_0\), \(\Delta V = V(P) - V_0\), and therefore

\[
R(P) = R_0[1 - 3P(S_{11} + 2S_{12})]^{1/3},
\] (31)

\[
L(P) = L_0[1 - 3P(S_{11} + 2S_{12})]^{1/3},
\] (32)

where \(R_0\) (\(L_0\)) is the radius (height) of the QD at atmospheric pressure, and \(S_{11}\) and \(S_{12}\) are the compliance constants of GaN given by\[30\]:

\[
S_{11} = \frac{(C_{11,GaN} + C_{12,GaN})}{[(C_{11,GaN} - C_{12,GaN})(C_{11,GaN} + 2C_{12,GaN})]},
\] (33)

\[
S_{12} = \frac{-C_{12,GaN}}{[(C_{11,GaN} - C_{12,GaN})(C_{11,GaN} + 2C_{12,GaN})]}.
\] (34)
3. Numerical results and discussion

We calculated the emission wavelengths and the electron-hole recombination rates in WZ GaN\textsubscript{Al\textsubscript{1-x}}\textsubscript{Ga\textsubscript{x}}\textsubscript{N} cylindrical QDs with finite height potential barriers by considering strain and hydrostatic pressure effects. For simplicity, we concentrated on the heavy-hole exciton states in the following. All the material parameters used in our calculations are listed in Tables 1–3.

A comparison between the theoretical and measured optical transition energies under zero hydrostatic pressure in GaN/Al\textsubscript{1-x}Ga\textsubscript{x}N QDs. For comparison, the results calculated by Dai et al. without considering the strain dependence of the material parameters are also listed.

### Table 1. Physical parameters of wurtzite GaN and AlN used in the computation.

<table>
<thead>
<tr>
<th></th>
<th>(a) (nm)</th>
<th>(C_{11}) (GPa)</th>
<th>(C_{12}) (GPa)</th>
<th>(C_{13}) (GPa)</th>
<th>(C_{33}) (GPa)</th>
<th>(e_{31}) (C/m²)</th>
<th>(e_{33}) (C/m²)</th>
<th>(P_{SP}) (C/m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaN</td>
<td>0.3189\textsuperscript{a}</td>
<td>390\textsuperscript{b}</td>
<td>145\textsuperscript{b}</td>
<td>106\textsuperscript{b}</td>
<td>398\textsuperscript{b}</td>
<td>-0.49\textsuperscript{c}</td>
<td>0.73\textsuperscript{c}</td>
<td>-0.029\textsuperscript{c}</td>
</tr>
<tr>
<td>AlN</td>
<td>0.3112\textsuperscript{a}</td>
<td>398\textsuperscript{b}</td>
<td>140\textsuperscript{b}</td>
<td>127\textsuperscript{b}</td>
<td>382\textsuperscript{b}</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\textsuperscript{a}Ref. [31]. \textsuperscript{b}Ref. [32]. \textsuperscript{c}Ref. [33].

### Table 2. The other physical parameters of wurtzite GaN and AlN used in the computation.

<table>
<thead>
<tr>
<th></th>
<th>(E_g) (meV)</th>
<th>(m_i^*(m_0))</th>
<th>(g) (meV/GPa)</th>
<th>(f_{lon})</th>
<th>(a_1) (meV)</th>
<th>(a_2) (meV)</th>
<th>(b_1) (meV)</th>
<th>(b_2) (meV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaN</td>
<td>3507\textsuperscript{a}</td>
<td>0.2\textsuperscript{a}</td>
<td>33\textsuperscript{b}</td>
<td>0.5\textsuperscript{b}</td>
<td>-4090\textsuperscript{d}</td>
<td>-8870\textsuperscript{d}</td>
<td>-7020\textsuperscript{d}</td>
<td>3650\textsuperscript{d}</td>
</tr>
<tr>
<td>AlN</td>
<td>6230\textsuperscript{a}</td>
<td>0.32\textsuperscript{a}</td>
<td>43\textsuperscript{b}</td>
<td>0.499\textsuperscript{c}</td>
<td>-3390\textsuperscript{d}</td>
<td>-11810\textsuperscript{d}</td>
<td>-9420\textsuperscript{d}</td>
<td>4020\textsuperscript{d}</td>
</tr>
</tbody>
</table>

\textsuperscript{a}Ref. [31]. \textsuperscript{b}Ref. [34]. \textsuperscript{c}Ref. [17]. \textsuperscript{d}Ref. [24].

### Table 3. The other physical parameters of wurtzite GaN and AlN used in the computation.

<table>
<thead>
<tr>
<th></th>
<th>(\varepsilon_{\infty, xx})</th>
<th>(\varepsilon_{\infty, zz})</th>
<th>(\alpha_{LO, xx}) (cm(^{-1}))</th>
<th>(\alpha_{LO, zz}) (cm(^{-1}))</th>
<th>(\alpha_{TO, xx}) (cm(^{-1}))</th>
<th>(\alpha_{TO, zz}) (cm(^{-1}))</th>
<th>(\gamma_{LO, xx})</th>
<th>(\gamma_{LO, zz})</th>
<th>(\gamma_{TO, xx})</th>
<th>(\gamma_{TO, zz})</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaN</td>
<td>5.20\textsuperscript{a}</td>
<td>5.39\textsuperscript{a}</td>
<td>757\textsuperscript{b}</td>
<td>748\textsuperscript{b}</td>
<td>568\textsuperscript{b}</td>
<td>541\textsuperscript{b}</td>
<td>0.99\textsuperscript{b}</td>
<td>0.98\textsuperscript{b}</td>
<td>1.19\textsuperscript{b}</td>
<td>1.21\textsuperscript{b}</td>
</tr>
<tr>
<td>AlN</td>
<td>4.30\textsuperscript{a}</td>
<td>4.52\textsuperscript{a}</td>
<td>924\textsuperscript{b}</td>
<td>898\textsuperscript{b}</td>
<td>677\textsuperscript{b}</td>
<td>618\textsuperscript{b}</td>
<td>0.91\textsuperscript{b}</td>
<td>0.82\textsuperscript{b}</td>
<td>1.18\textsuperscript{b}</td>
<td>1.02\textsuperscript{b}</td>
</tr>
</tbody>
</table>

\textsuperscript{a}Ref. [24]. \textsuperscript{b}Ref. [14].

### Table 4. Calculated and measured optical transition energies under zero hydrostatic pressure in GaN/Al\textsubscript{1-x}Ga\textsubscript{x}N QDs. For comparison, the results calculated by Dai et al. without considering the strain dependence of the material parameters are also listed.

<table>
<thead>
<tr>
<th></th>
<th>(L) (nm)</th>
<th>(R) (nm)</th>
<th>(x)</th>
<th>(E_{ph}^{exp}(eV))</th>
<th>(E_{ph}^{calc}(eV))</th>
<th>(\text{Error (%)})</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>3.5</td>
<td>5</td>
<td>0.15</td>
<td>3.581\textsuperscript{a}</td>
<td>3.560</td>
<td>0.59 2\textsuperscript{b}</td>
</tr>
<tr>
<td></td>
<td>5.5</td>
<td>25</td>
<td>0.10</td>
<td>3.440\textsuperscript{c}</td>
<td>3.443</td>
<td>0.09 0.7\textsuperscript{b}</td>
</tr>
</tbody>
</table>

\textsuperscript{a}Ref. [19]. \textsuperscript{b}Ref. [10]. \textsuperscript{c}Ref. [35].
recombination rate greatly. Comparing curve B with curve D, we note that the strain dependence of the material parameters induces the increase in the recombination rate and has a remarkable influence for the QDs with a small L height.

In Fig. 3, the emission wavelength $\lambda$ and the electron–hole recombination rate are further investigated as a function of Al content $x$ in GaN/Al$_x$Ga$_{1-x}$N QDs with height $L = 2$ nm and radius $R = 5$ nm under zero hydrostatic pressure. Curve A is with built-in electric field and strain dependence of the physical parameters, curve B is without strain effect, curve C is only with built-in electric field, and curve D is only with strain dependence of the physical parameters. Comparing curve B with curve C in Fig. 3(a), we can see that the strong BEF gives rise to an increase in the emission wavelength when the Al content is increased. Figure 3(a) also shows that the strain dependence of the material parameters leads to a large decrease in the emission wavelength, and has a remarkable influence on the QDs with large Al content (see curves B and D). The interaction of these two effects induces the emission wavelength with strain effect to become lower than that without strain effect, especially for the QDs with a large Al content (see curves A and B). This result coincides with the one obtained from Fig. 2(a). In particular, from Fig. 3(b) we can clearly see that the BEF greatly reduces the electron-hole recombination rate (see curves B and C). And the strain dependence of the material parameters obviously increases the recombination rate when the Al content is less (see curves B and D). The interaction of these two effects slowly diminishes the electron-hole recombination rate with strain effect, with increasing Al content (curve A).

Figure 4 gives the emission wavelength $\lambda$ in strained WZ GaN/Al$_{0.15}$Ga$_{0.85}$N cylindrical QDs as a function of the hydrostatic pressure. It shows that the emission wavelength linearly decreases with increasing hydrostatic pressure. The pressure-related changes are mainly due to the pressure dependence of both the energy gap of GaN and the QD volume. The behav-
The interaction of these two effects leads to an emission wavelength increase and an increase in the electron–hole recombination rate. The material parameters lead to a decrease in the emission wavelength and an increase in the electron–hole recombination rate. The strong BEF gives rise to an increase in the emission wavelength and a large reduction in the electron–hole recombination rate. The interaction of these two effects leads to an emission wavelength with strain effect that is higher than without strain effect even when the QD height is > 3.8 nm, but the opposite of this occurs when the QD height is < 3.8 nm. The height of GaN QDs must be less than 5.5 nm for an efficient electron–hole recombination process due to the strain effect. The emission wavelength decreases linearly and the electron–hole recombination rate increases almost linearly with applied hydrostatic pressure. The hydrostatic pressure has a remarkable influence on the emission wavelength for large QDs, and a significant influence on the electron–hole recombination rate for small QDs. Furthermore, our numerical outcomes are in qualitative agreement with previous experimental findings under zero pressure.

4. Conclusions

We investigated the effects of strain and hydrostatic pressure on the emission wavelength and electron–hole recombination rate in wurtzite GaN/Al$_{x}$Ga$_{1-x}$N cylindrical QDs with finite potential barriers. Calculations are performed via a variational procedure within the effective-mass approximation. Numerical results show that the strain dependence of the material parameters leads to a decrease in the emission wavelength and an increase in the electron–hole recombination rate. The strong BEF gives rise to an increase in the emission wavelength and a large reduction in the electron–hole recombination rate. The interaction of these two effects leads to an emission wavelength with strain effect that is higher than without strain effect even when the QD height is > 3.8 nm, but the opposite of this occurs when the QD height is < 3.8 nm. The height of GaN QDs must be less than 5.5 nm for an efficient electron–hole recombination process due to the strain effect. The emission wavelength decreases linearly and the electron–hole recombination rate increases almost linearly with applied hydrostatic pressure. The hydrostatic pressure has a remarkable influence on the emission wavelength for large QDs, and a significant influence on the electron–hole recombination rate for small QDs. Furthermore, our numerical outcomes are in qualitative agreement with previous experimental findings under zero pressure.

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Fig. 5. Electron–hole recombination rate in strained GaN/Al$_{0.15}$Ga$_{0.85}$N QDs as a function of the hydrostatic pressure for different QD sizes.


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