Binding energies of excitons in a strained wurtzite GaN/AlGaN quantum well influenced by screening and hydrostatic pressure

2008 J. Phys.: Condens. Matter 20 085218

(http://iopscience.iop.org/0953-8984/20/8/085218)

IOP Publishing — Journal of Physics: Condensed Matter

J. Phys.: Condens. Matter **20** (2008) 085218 (7pp) — doi:10.1088/0953-8984/20/8/085218

Binding energies of excitons in a strained wurtzite GaN/AlGaN quantum well influenced by screening and hydrostatic pressure

S H Ha and S L Ban

Department of Physics, College of Sciences and Technology, Inner Mongolia University,
Hohhot 010021, People's Republic of China

E-mail: slban@imu.edu.cn

Received 26 October 2007, in final form 16 January 2008
Published 1 February 2008
Online at stacks.iop.org/JPhysCM/20/085218

Abstract

In the framework of effective mass and single-band approximations, a variational method combined with a self-consistent procedure is adopted to discuss the binding energies of heavy-hole excitons in a strained wurtzite GaN/$Al_{0.3}Ga_{0.7}N$ quantum well by considering the hydrostatic pressure effect and screening due to the electron–hole gas. The built-in electric field in such a structure produced by spontaneous polarization and strain-induced piezoelectric polarization is considered in our calculation. A simplified coherent potential approximation is extended to calculate the energy gaps of the ternary mixed crystal $Al_xGa_{1-x}N$. The result indicates that the binding energies of excitons increase nearly linearly with pressure even when taking into consideration the modification of strain. It is also found that the percentage increase of the binding energy with pressure is influenced by the electron–hole density due to the influence of pressure on the screening and exclusion effects. The excitonic binding energies increase obviously with decreasing barrier thickness due to the built-in electric field.

1. Introduction

In recent decades, low-dimensional structures made of wurtzite group-III nitride semiconductors such as AlN, GaN and InN have attracted much attention due to their promising applications in short-wavelength electroluminescence devices, such as light-emitting diodes (LED) and laser diodes (LDs) [1–3]. In particular, it is known that a large spontaneous polarization and strain-induced piezoelectric polarization are present in these relatively low-symmetry wurtzite structures to play an important role in determining the optical and electrical properties via polarization-induced built-in electric fields [4, 5].

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. Wagner *et al* [6] presented *ab initio* calculations of the structural, dielectric and lattice-dynamical properties of zinc-blende and wurtzite GaN and AlN under hydrostatic pressure. Gõni *et al* [7] investigated experimentally the pressure modification of the phonon modes in wurtzite (hexagonal) and zinc-blende (cubic) GaN and wurtzite AlN. Łepkowski *et al* [8] 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 pressure dependence of the peak photoluminescence energy was reduced with respect to the pressure dependence of the energy gap; this could be explained by the hydrostatic pressure-induced increase of the piezoelectric field in the quantum structures. In a similar way, Vaschenko *et al* [9] explored the dominant role of the piezoelectric field under pressure for InGaN/GaN quantum wells (QWs) and obtained two important conclusions: (1) a strong effect of the built-in piezoelectric field on the emission characteristics of InGaN/GaN QWs under hydrostatic pressure was shown; (2) an increase of the piezoelectric field with hydrostatic pressure was explained by the significant dependence of the InGaN piezoelectric constants on strain.

0953-8984/08/085218+07$30.00

Usually, the pressure effect on GaAs/Al$_x$Ga$_{1-x}$As heterostructures may be simple since the strain can be neglected due to the interface lattice matching. Using a linear interpolation and variation method, Ban *et al* [10] studied the pressure effect on the binding energies of donors in a realistic GaAs/Al$_x$Ga$_{1-x}$As heterojunction. More recently, the binding energies of excitons in a GaAs/AlAs QW were investigated [11]. Then, they [12] calculated the binding energies of donors in QWs under pressure for GaAs/Al$_x$Ga$_{1-x}$As and zinc-blende GaN/Al$_x$Ga$_{1-x}$N structures (without strain), respectively. Their results showed that pressure obviously enhances the binding energies of donors and excitons. On the other hand, Bigenwald *et al* [13, 14] calculated the exciton states assuming the presence of an electron–hole (EH) plasma created by photoexcited carriers, and obtained a non-monotonic behavior of the exciton binding energy as a function of the EH density. Unfortunately, the kinetic energy of an EH pair dissociated from an exciton was neglected in their calculation of the binding energy. More recently, Kalliakos *et al* [15] investigated the effects of large EH pair density on the excitonic energy spectra of hexagonal group-III nitride QWs such as GaN/Al$_x$Ga$_{1-x}$N or In$_y$Ga$_{1-y}$N/GaN, by solving self-consistently the Schrödinger and Poisson equations to calculate the charges of emission and absorption spectra induced by the screening of the large internal electric field.

However, the influence of screening, due to the two-dimensional free EH gas, on the binding energies of heavy-hole excitons in strained QWs under the hydrostatic pressure has not been investigated. This motivated us to discuss the pressure effect on the binding energies of heavy-hole excitons confined in a strained wurtzite GaN/AlGaN QW. The thickness effect of barriers is also considered here. Furthermore, the influence of Fermi energy as a function of EH density on the binding energy is considered here to improve upon the previous works [13, 14]. Within the framework of effective mass and the single-band approximation, the results indicate that pressure obviously increases the excitonic stability, and the percentage increase of the binding energy with pressure is influenced by the EH density. Moreover, it was found that the excitonic binding energies increase as the barrier thickness decreases due to the built-in electric field. This effect is opposite to the quantum confinement effect of a QW.

2. Theory and calculation

In the following, the Schrödinger equation is introduced first, followed by a discussion of the pressure and strain dependence of the parameters (band gap, effective mass and static electric field) in this equation. The Poisson equation for the self-consistent potential is then presented, and the pressure together with strain dependence of the dielectric constant is discussed. Finally the variational ansatz for the wavefunction is given, and the calculation of binding energy is described.

2.1. Schrödinger equation

A strained wurtzite GaN/Al$_{0.3}$Ga$_{0.7}$N QW with finite height barriers under the influence of a two-dimensional (2D) EH gas is considered to calculate the binding energies of heavy-hole excitons as functions of the EH density under hydrostatic pressure. The 2DEH gas is created by photoexcited carriers to induce a transverse electric field. Moreover, the biaxially and uniaxially strained QW excites large built-in electric fields. Without loss of generality, the interfaces of the QW are chosen as parallel to the x–y plane with the well center at the zero point in the z direction.

It is obvious that the motion of carriers in the z direction is quantized and can be separated from the plane wave in the x–y direction. To determine the ground state for electrons (holes) in a QW in the z direction, a self-consistent procedure is adopted by solving both the Schrödinger and Poisson equations [13]. The Schrödinger equation for an electron (hole) in the growth direction z can be written as

$$\left\{-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\left[\frac{1}{m_{\rm j}^{\perp}(z)}\frac{\partial}{\partial z}\right]+V_{\rm j}(z)+q_{\rm j}[F(z)+\varphi_{\rm j}(z)]z\right\}\psi_{\rm j}(z)$$
$$=E_{\rm j}\psi_{\rm j}(z), \qquad (1)$$

where the superscript j = e, h denotes the electron and hole, respectively. The charge $q_{\rm j}$ is e for an electron and −e for a hole, respectively.

2.2. Pressure and strain dependence of parameters in the Schrödinger equation

In the strained wurtzite nitride QW, the ratio of the conduction band to the valence band offset is given to be 65:20 [16]. Then, the strain-affected band offsets are given as

$$V_{\rm e}(z)=\begin{cases}0 & \text{in well}\\ V_{0,\rm e}=0.765(E_{\rm g,b}-E_{\rm g,w}) & \text{in barriers,}\end{cases} \qquad (2)$$

$$V_{\rm h}(z)=\begin{cases}0 & \text{in well}\\ V_{0,\rm h}=0.235(E_{\rm g,b}-E_{\rm g,w}) & \text{in barriers.}\end{cases} \qquad (3)$$

In the above equations, the pressure- and strain-dependent energy gaps [17] of GaN and AlN are

$$E_{\rm g,w}=E_{\rm g,w}(p)+2(d_{1,\rm w}+b_{1,\rm w})\varepsilon_{xx,\rm w}+(d_{2,\rm w}+b_{2,\rm w})\varepsilon_{zz,\rm w}, \qquad (4)$$

$$E_{\rm g,b(AlN)}=E_{\rm g,b(AlN)}(p)+2d_{1,\rm b}\varepsilon_{xx,\rm b}+d_{2,\rm b}\varepsilon_{zz,\rm b}, \qquad (5)$$

where $d_{1,\rm i}$, $d_{2,\rm i}$, $b_{1,\rm i}$ and $b_{2,\rm i}$ are the deformation potentials, for which the superscript i = w, b donates the well and barrier materials, respectively. The dependence of the energy gap on hydrostatic pressure p is considered by the following equation [18]

$$E_{\rm g,i}(p)=E_{\rm g,i}+\alpha_{\rm i}p. \qquad (6)$$

Here, we extend a simplified coherent potential approximation [19] to calculate the energy gap of ternary mixed crystal Al$_x$Ga$_{1-x}$N (chosen as the barriers):

$$E_{\rm g,b}=\frac{E_{\rm g,w}E_{\rm g,b(AlN)}}{xE_{\rm g,w}+(1-x)E_{\rm g,b(AlN)}}. \qquad (7)$$

In the well and barriers, the biaxial lattice-mismatch-induced strains are given as

$$\varepsilon_{xx,\rm w}=\varepsilon_{yy,\rm w}=\frac{a_{\rm eq}(p)-a_{\rm w}(p)}{a_{\rm w}(p)}, \qquad (8)$$

and

$$\varepsilon_{xx,\mathrm{b}} = \varepsilon_{yy,\mathrm{b}} = \frac{a_{\mathrm{eq}}(p) - a_{\mathrm{b}}(p)}{a_{\mathrm{b}}(p)}, \tag{9}$$

where a_{eq} represents the equilibrium, or actual, lattice constant for the strained layer. It is given by [20]

$$a_{\mathrm{eq}}(p) = \frac{a_{\mathrm{w}}(p)L_{\mathrm{w}} + a_{\mathrm{b}}(p)L_{\mathrm{b}}}{L_{\mathrm{w}} + L_{\mathrm{b}}}. \tag{10}$$

For infinitely thick barriers ($L_{\mathrm{b}} \to \infty$), it is replaced by $a_{\mathrm{eq}} = a_{\mathrm{b}}$.

The lattice constant as a function of hydrostatic pressure [21] is given by

$$a_{\mathrm{i}}(p) = a_{\mathrm{i}}(0)\left(1 - \frac{p}{3B_{0,\mathrm{i}}}\right). \tag{11}$$

The bulk modulus in a wurtzite structure is given by the elastic constants C_{11}, C_{12}, C_{13} and C_{33} as

$$B_{0,\mathrm{i}} = \frac{(C_{11,\mathrm{i}} + C_{12,\mathrm{i}})C_{33,\mathrm{i}} - 2C_{13,\mathrm{i}}^2}{C_{11,\mathrm{i}} + C_{12,\mathrm{i}} + 2C_{33,\mathrm{i}} - 4C_{13,\mathrm{i}}}. \tag{12}$$

The stress tensors $\varepsilon_{xx,\mathrm{i}}$ and $\varepsilon_{zz,\mathrm{i}}$ under hydrostatic pressure are equal, and from Hooke's law the uniaxial and biaxial strain tensor ratio can be expressed by [22]

$$\frac{\varepsilon_{zz,\mathrm{i}}}{\varepsilon_{xx,\mathrm{i}}} = \frac{C_{11,\mathrm{i}} + C_{12,\mathrm{i}} - 2C_{13,\mathrm{i}}}{C_{33,\mathrm{i}} - C_{13,\mathrm{i}}}. \tag{13}$$

Following the above procedure for determining energy gaps, the biaxial, uniaxial and hydrostatic pressure dependences of the effective masses of an electron [23] in the z direction and the x–y plane can be calculated by

$$\frac{m_0}{m_{\mathrm{e,i}}^{\perp,\parallel}(p)} = 1 + \frac{C}{E_{\mathrm{g,i}}(p)}. \tag{14}$$

Here C is a constant and can be determined by solving equation (14) at $p = 0$. In general, the pressure coefficient for a heavy-hole is assumed to be zero.

In equation (1), the internal electric field $F(z)$ is different in the well and barrier materials. To calculate it, the spontaneous and piezoelectric polarizations must be considered in a wurtzite structure as follows [8]:

$$F_{\mathrm{w}} = \frac{L_{\mathrm{b}}(P_{\mathrm{b}}^{\mathrm{pz}} + P_{\mathrm{b}}^{\mathrm{sp}} - P_{\mathrm{w}}^{\mathrm{pz}} - P_{\mathrm{w}}^{\mathrm{sp}})}{L_{\mathrm{b}}\kappa_{0\mathrm{w}} + L_{\mathrm{w}}\kappa_{0\mathrm{b}}}, \tag{15}$$

and

$$F_{\mathrm{b}} = \frac{L_{\mathrm{w}}(P_{\mathrm{w}}^{\mathrm{pz}} + P_{\mathrm{w}}^{\mathrm{sp}} - P_{\mathrm{b}}^{\mathrm{pz}} - P_{\mathrm{b}}^{\mathrm{sp}})}{L_{\mathrm{b}}\kappa_{0\mathrm{w}} + L_{\mathrm{w}}\kappa_{0\mathrm{b}}}, \tag{16}$$

where the data of spontaneous polarization $P_{\mathrm{i}}^{\mathrm{sp}}$ (i = b, w) were given in [24], and the strain-induced piezoelectric polarizations are written as [8]:

$$P_{\mathrm{i}}^{\mathrm{pz}} = 2e_{31,\mathrm{i}}\varepsilon_{xx,\mathrm{i}} + e_{33,\mathrm{i}}\varepsilon_{zz,\mathrm{i}}, \tag{17}$$

where $e_{31,\mathrm{i}}$ and $e_{33,\mathrm{i}}$ are the strain-dependent piezoelectric constants satisfying [9]

$$e_{31,\mathrm{i}} = e_{31,\mathrm{i}}^{(0)} + \frac{4eZ_{\mathrm{i}}}{\sqrt{3}a_{\mathrm{i}}^2}\frac{\mathrm{d}u_{\mathrm{i}}}{\mathrm{d}\varepsilon_{xx,\mathrm{i}}}, \tag{18}$$

and

$$e_{33,\mathrm{i}} = e_{33,\mathrm{i}}^{(0)} + \frac{4eZ_{\mathrm{i}}}{\sqrt{3}a_{\mathrm{i}}^2}\frac{\mathrm{d}u_{\mathrm{i}}}{\mathrm{d}\varepsilon_{zz,\mathrm{i}}}. \tag{19}$$

For infinitely wide barriers, the built-in electric filed in the barriers will vanish, whereas F_{w} can be obtained by equation (15) with the limit of $L_{\mathrm{b}} \to \infty$.

2.3. *Poisson equation*

In equation (1), the free-carrier-induced field $\varphi_{\mathrm{j}}(z)$ can be obtained by solving the Poisson equation

$$\varphi_{\mathrm{j}}(z + \mathrm{d}z) - \varphi_{\mathrm{j}}(z) = q_{\mathrm{j}}N_s \int_z^{z+\mathrm{d}z} f(u)\frac{\mathrm{d}u}{\kappa_{0,zz}(u)}, \tag{20}$$

where $f(u) = \psi_{\mathrm{e}}^2(u) - \psi_{\mathrm{h}}^2(u)$. $\kappa_{0,zz}(u)$ is the static dielectric constant of material dependence, and N_s is the EH density. Here, the single particle (electron or hole) energy level E_{j} and wavefunction $\psi_{\mathrm{j}}(z)$ can be obtained by solving equations (1) and (20) self-consistently.

The Hamiltonian for an exciton can be written as

$$H_{\mathrm{e-h}} = -\frac{\hbar^2}{2\mu_{\mathrm{e-h}}}\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) + e\varphi_{\mathrm{e-h}}(z_{\mathrm{e}}, z_{\mathrm{h}}, \rho), \tag{21}$$

where ρ is the distance between the electron and hole in the x–y plane, and $\mu_{\mathrm{e-h}} = m_{\mathrm{e}}^{\parallel}m_{\mathrm{h}}^{\parallel}/(m_{\mathrm{e}}^{\parallel} + m_{\mathrm{h}}^{\parallel})$ is the reduced mass of the exciton, in which $m_{\mathrm{e}}^{\parallel}$ and $m_{\mathrm{h}}^{\parallel}$ are the effective masses of the electron and hole parallel to the x–y plane, respectively. The screened Coulombic potential [13, 14] is given in the representation of the resultant mixed (z, q) by

$$e\varphi_{\mathrm{e-h}}(z_{\mathrm{e}}, z_{\mathrm{h}}, q) = \frac{e^2}{4\pi\kappa_0 q} \times \left\{\mathrm{e}^{-q|z_{\mathrm{e}}-z_{\mathrm{h}}|} - \frac{[\int \mathrm{d}u\, \mathrm{e}^{-q|u-z_{\mathrm{e}}+z_{\mathrm{h}}|} f(u)]^2}{\frac{q}{q_s} + \int \mathrm{d}u\, f(u)\int \mathrm{d}u'\, f(u')\mathrm{e}^{-q|u-u'|}}\right\}, \tag{22}$$

where $q_{\mathrm{s}} = 2\mu e^2/4\pi\kappa_0\hbar^2$ is the reciprocal screening radius. A variational method will be used later to calculate the variational energy of the exciton.

2.4. *Pressure and strain dependence of the dielectric constants*

In equation (22), the static dielectric constant κ_0 is influenced by the biaxial, uniaxial and hydrostatic pressures, respectively. The tensor components of κ_0 for the wurtzite structure are derived from the generalized Lyddane–Sachs–Teller relation

$$\kappa_{0,\alpha\alpha} = \kappa_{\infty,\alpha\alpha}\left(\frac{\omega_{\mathrm{LO},\alpha\alpha}}{\omega_{\mathrm{TO},\alpha\alpha}}\right)^2. \tag{23}$$

The frequencies of LO- and TO-phonons influenced by pressure and strain can be written as [22]

$$\omega_{j,\alpha\alpha} = \omega_{j,\alpha\alpha}(p) + 2K_{j,xx}\varepsilon_{xx} + K_{j,zz}\varepsilon_{zz}, \tag{24}$$

where $K_{j,xx}$ and $K_{j,zz}$ are the strain coefficients of phonon modes given in [22]. The tensor component ($\alpha = z, x$) is

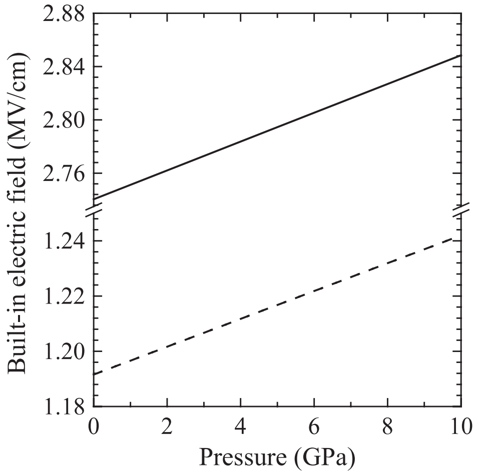

Figure 1. Built-in electric fields as functions of the hydrostatic pressure in QWs with infinite (solid line) and finite thickness (dashed line) barriers, respectively.

related to the LO- and TO-phonon frequencies, respectively. Furthermore, the hydrostatic pressure dependence of $\omega_{j,\alpha\alpha}(p)$ can be determined by the given mode Grüneisen parameter

$$\gamma_{j,\alpha\alpha} = B_0 \frac{1}{\omega_{j,\alpha\alpha}} \frac{\partial \omega_{j,\alpha\alpha}(p)}{\partial p}. \tag{25}$$

Considering the influence of hydrostatic pressure, biaxial and uniaxial strains, the high frequency dielectric constant in equation (23) can be rewritten as [25]

$$\frac{\partial \kappa_{\infty,\alpha\alpha}(p)}{\partial p} = -\frac{5(\kappa_{\infty,\alpha\alpha} - 1)}{3B_0}(0.9 - f_{\mathrm{ion}}), \tag{26}$$

where f_{ion} is the ionicity of the material under pressure.

2.5. Variational ansatz and binding energy

A one-parameter trial wavefunction in the x–y plane for an exciton taking into account the filling of the reciprocal space below the Fermi level was determined by Pikus [26]

$$\psi(\rho) = A\mathrm{e}^{-\beta\rho}\cos(k_{\mathrm{F}}\rho), \tag{27}$$

where k_{F} is the Fermi vector defined by $k_{\mathrm{F}} = \sqrt{2\pi N_s}$ at zero temperature [27].

Combining equations (1) and (21) with (27), the variational energy of an exciton in the ground state can be written as

$$E_{\mathrm{e-h}} = \langle\psi|H_{\mathrm{e-h}}|\psi\rangle$$
$$= \int \mathrm{d}z_{\mathrm{e}}\,|\psi_{\mathrm{e}}(z_{\mathrm{e}})|^2 \int \mathrm{d}z_{\mathrm{h}}\,|\psi_{\mathrm{h}}(z_{\mathrm{h}})|^2 \int \mathrm{d}^2\rho\,\psi^*(\rho)H_{\mathrm{e-h}}\psi(\rho). \tag{28}$$

Then the total variational energy is given by

$$E(\beta) = \sum_{j=\mathrm{e,h}} E_{\mathrm{j}} + E_{\mathrm{e-h}}. \tag{29}$$

As a result, the excitonic binding energy for the ground state can be written as

$$E_{\mathrm{b}} = E_{\mathrm{free}} - E, \tag{30}$$

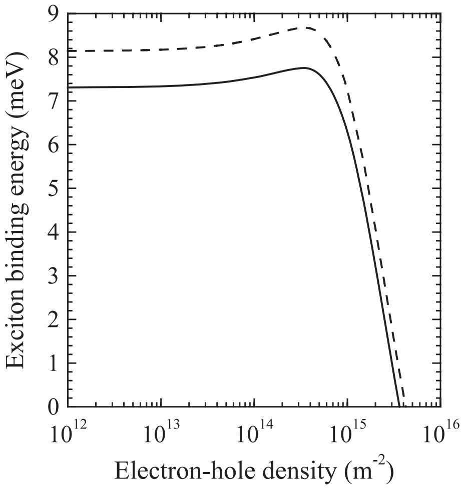

Figure 2. Binding energies of excitons screened by the EH gas in the strained GaN/$\mathrm{Al_{0.3}Ga_{0.7}N}$ QWs with infinite (solid line) and finite (dashed line) thickness barriers as functions of the EH density under 0 GPa, respectively.

where E is the ground state energy of the exciton and can be obtained by minimizing $E(\beta)$ with respect to β. E_{free} is the ground state energy of the free electron and hole, which can be obtained by repeating the above process but removing the Coulombic potential in equation (21) and replacing equation (27) by $\psi(\rho_{\mathrm{i}}) = \mathrm{e}^{\mathrm{i}\vec{k}_{\mathrm{F}}\cdot\vec{\rho}_{\mathrm{i}}}/2\pi$ for the electron (i = e) and hole (i = h). Then the energy for free-carriers is given as

$$E_{\mathrm{free}} = \sum_{\mathrm{i=e,h}} E_{\mathrm{i}} + E_{\mathrm{Fermi}}, \tag{31}$$

where the Fermi energy is as follows:

$$E_{\mathrm{Fermi}} = \frac{\hbar^2 k_{\mathrm{F}}^2}{2m_{\mathrm{e}}^{\parallel}} + \frac{\hbar^2 k_{\mathrm{F}}^2}{2m_{\mathrm{h}}^{\parallel}} = \frac{\hbar^2 k_{\mathrm{F}}^2}{2\mu_{\mathrm{e-h}}}. \tag{32}$$

The contribution given by equation (32) for free electron and hole energies was ignored in [13, 14] when the authors calculated the binding energy. The QW contains the EH carriers occupying the lower QW subbands; thus the kinetic energy of the unbound EH pair can be estimated as the energies at the Fermi levels to correct E_{b} by equation (30).

3. Results and discussion

In this section, the binding energies of heavy-hole excitons in a biaxially and uniaxially strained wurtzite GaN/$\mathrm{Al_{0.3}Ga_{0.7}N}$ QW are computed by considering hydrostatic pressure effect and screening due to the EH gas. The parameters used in our computation are listed in tables 1–3. The calculated results are shown in figures 1–5, respectively.

Figure 1 shows the increases in the built-in electric field as the hydrostatic pressure for QWs with infinite and finite thickness barriers, respectively. Without losing generality, the finite thickness of barriers is taken to be equal to the thickness of a well (50 Å) to see the thickness effect of barriers. The calculated built-in electric fields in the well and barriers are

Table 1. Physical parameters of wurtzite GaN and AlN used in the computation. The parameters of $Al_xGa_{1-x}N$ were calculated with the linear interpolation method. The lattice constants are in units of angstroms, piezoelectric constants in C m^{-2}, the elastic constants in GPa, and the spontaneous polarization in C m^{-2}, respectively.

	a	C_{11}	C_{12}	C_{13}	C_{33}	u	Z	$e_{31}^{(0)}$	$e_{33}^{(0)}$	P^{sp}
GaN	3.189[a]	390[a]	145[a]	106[a]	398[a]	0.377[b]	1.18[b]	−0.49[c]	0.73[c]	−0.029[c]
AlN	3.122[a]	398[a]	140[a]	127[a]	382[a]	0.382[b]	1.27[b]	−0.60[c]	1.46[c]	−0.081[c]

[a] Reference [28].
[b] Reference [22].
[c] Reference [24].

Table 2. Physical parameters of wurtzite GaN and AlN used in the computation. The energy gaps and deformation potentials are in units of meV, and the effective masses in the bare electron mass m_0, respectively.

	E_g	d_1	d_2	b_1	b_2	α	$m_e^{\perp}$	$m_e^{\parallel}$	$m_h^{\perp}$	$m_h^{\parallel}$
GaN	3390[a]	−4090[b]	−8870[b]	−7020[b]	3650[b]	3.3[c]	0.19[d]	0.23[d]	0.37[e]	2.09[e]
AlN	6200[a]	−3390[b]	−1180[b]	−9420[b]	4020[b]	4.3[c]	0.33[e]	0.32[e]	0.73[e]	3.52[e]

[a] Reference [29].
[b] Reference [22].
[c] Reference [30].
[d] Reference [31].
[e] Reference [32].

Table 3. Physical parameters of wurtzite GaN and AlN used in the computation. The frequencies are in units of cm^{-1}.

	$\kappa_{\infty,xx}$	$\kappa_{\infty,zz}$	$\omega_{LO,xx}$	$\omega_{LO,zz}$	$\omega_{TO,xx}$	$\omega_{TO,zz}$	$\gamma_{LO,xx}$	$\gamma_{LO,zz}$	$\gamma_{TO,xx}$	$\gamma_{TO,zz}$	f_{ion}
GaN	5.20[a]	5.39[a]	757[b]	748[b]	568[b]	540[b]	0.91[b]	0.82[b]	1.18[b]	1.02[b]	0.5[c]
AlN	4.30[a]	4.52[a]	924[b]	898[b]	677[b]	618[b]	0.99[b]	0.98[b]	1.19[b]	1.21[b]	0.499[c]

[a] Reference [22].
[b] Reference [6].
[c] Reference [33].

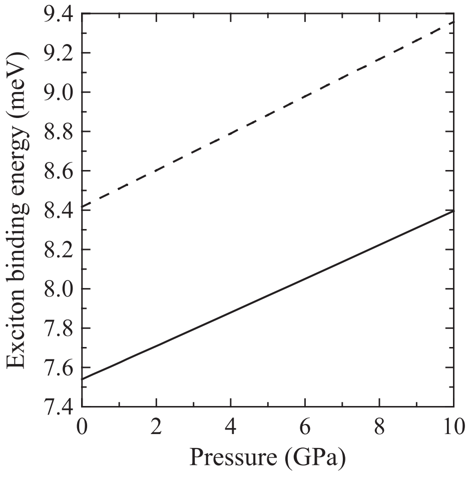

Figure 3. Binding energies of excitons in the strained $GaN/Al_{0.3}Ga_{0.7}N$ QWs with infinite (solid line) and finite thickness (dashed line) barriers as functions of the pressure under EH density 1×10^{14} m^{-2}, respectively.

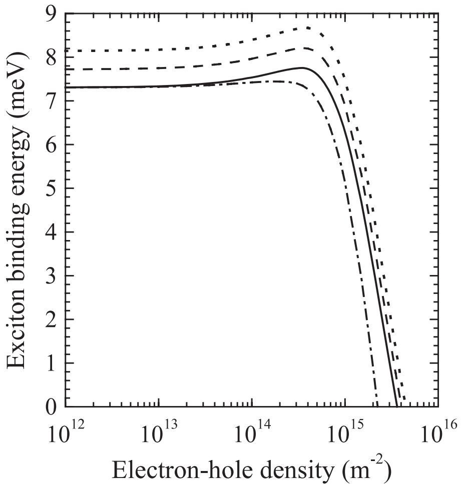

Figure 4. Binding energies of excitons in strained $GaN/Al_{0.3}Ga_{0.7}N$ QWs with infinite thickness barriers as functions of the EH densities under pressures of 0 (solid line), 5 (dashed line) and 10 GPa (dotted line), respectively. The dash–dotted line represents the binding energies of excitons defined in [13, 14] as a function of the EH density.

equal, whereas the field in the well is negative and opposite to the growth direction of the QW, and the field in the barriers is positive and along the growth direction. Moreover, the absolute values for both cases increase with the hydrostatic pressure. When the barrier is assumed to be infinitely thick, the built-in electric field in the barriers will vanish. It can be seen that the thickness of the barriers obviously influences the built-in electric field. The pressure effect on the field varying with

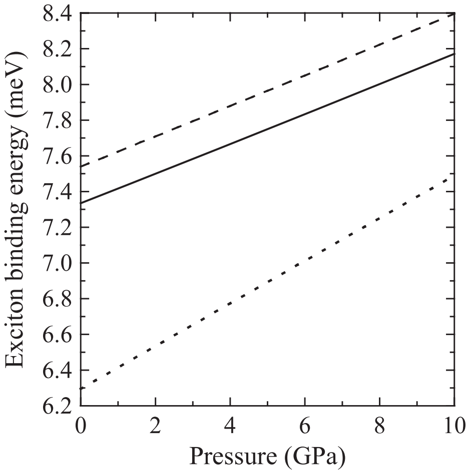

Figure 5. Binding energies of excitons in the strained GaN/$Al_{0.3}Ga_{0.7}N$ QWs with infinite thickness barriers as functions of the pressure under the EH densities of 1×10^{13} m^{-2} (solid line), 1×10^{14} m^{-2} (dashed line) and 1×10^{15} m^{-2} (dotted line), respectively.

thickness of the barriers is insensitive since the increases of the built-in electric fields are 3.95% and 4.23%, respectively, for infinite and finite thickness barriers as pressure increases from 0 to 10 GPa.

Figure 2 shows the binding energies of excitons screened by the EH gas in the strained QWs with infinite and finite thickness barriers as functions of the EH density, respectively. The result indicates that binding energies of excitons in the two cases both first increase slowly to a maximum with increasing density of EH gas and then decrease rapidly when the density is larger than about 1×10^{15} m^{-2}. It is clearly seen that the binding energy of the exciton in a QW with finite thickness barriers is larger than that in a QW with infinite thickness barriers because of the smaller built-in electric field for the former. The electric field will separate the electron and hole in opposite directions to decrease the excitonic binding energy, and the larger (wider barriers) the electric field is, the lower the binding energy. The field in a QW with infinite thickness barriers is nearly twice as large as the finite ones, and the binding energy decreases by 11.4% compared with the latter one. This effect may weaken the quantum confinement effect of a QW. For a larger EH density, the thickness effect of barriers decreases somewhat since the competition from screening of the EH gas increases rapidly.

Figure 3 gives the binding energies of excitons in the strained QWs with infinite and finite thickness barriers, respectively, as functions of the hydrostatic pressure. It shows that the binding energies of the excitons increase nearly linearly on increasing the pressure in QWs with both infinite and finite thickness barriers. The finite thickness of barriers increases the binding energy by 11.6% with respect to the infinite case.

Figure 4 shows the binding energies of excitons in a strained GaN/$Al_{0.3}Ga_{0.7}N$ QW as functions of the EH densities under different pressures, for which the thickness of the barrier is adopted to be infinite. The changing tendency of the exciton binding energies with the EH density at 5 and 10 GPa is similar to that at zero pressure. It shows that the binding energy is more stable for a low EH density, and increases beginning from some EH density and then slowly reaching a maximum. The result agrees qualitatively with the conclusion in [14]. The binding energies of excitons defined in [13, 14] as a function of the EH density under zero pressure are also shown in the figure. It can be clearly seen that the difference between the binding energies with the two different definitions becomes obvious for higher EH densities because the rise (drop) of the Fermi level for the electron (hole) is more remarkable with increasing EH density. Thus, the ratio of the difference in the binding energy (defined in [13, 14]) increases from 0.02% to 22.5% for EH density from 1×10^{12} to 1×10^{15} m^{-2}. It should be pointed out that the Pikus ansatz is unsuitable for a very higher EH density near which the exciton collapses [34].

Figure 5 shows the binding energies of excitons in a strained GaN/$Al_{0.3}Ga_{0.7}N$ QW with a finite thickness barrier calculated as functions of the pressures for EH densities of 1×10^{13}, 1×10^{14} and 1×10^{15} m^{-2}, respectively. The result indicates that the binding energies of excitons increase nearly linearly on increasing the pressure for a given EH density. As pressure increases from 0 to 10 GPa, the binding energy increases by about 11.41%, 11.36% and 18.98% for EH densities of 1×10^{13} m^{-2}, 1×10^{14} m^{-2} and 1×10^{15} m^{-2}, respectively. The exciton binding energy as a function of EH density was explained in [13, 14] at zero pressure, whereas pressure has a slight influence on 'the screening and exclusion effects' at lower EH densities but decreases the effects dramatically at an EH density of $\geqslant 1 \times 10^{15}$ m^{-2}. Together with figure 4, it is seen that the pressure obviously increases the excitonic stability and lowers the maximum points slightly.

4. Summary

In summary, the binding energies of heavy-hole excitons in a biaxially and uniaxially strained wurtzite GaN/$Al_{0.3}Ga_{0.7}N$ QW are discussed by considering the hydrostatic pressure effect and screening due to the EH gas. A variational method and a self-consistent procedure are combined to calculate the binding energies influenced by the spontaneous polarization and strain-induced piezoelectric polarization-induced built-in electric fields, which is enhanced by the pressure. The result indicates that the binding energies of excitons increase nearly linearly with pressure, even the modification of strain with hydrostatic pressure is considered and the percentage increase of the binding energy with pressure is influenced by the EH density. The pressure obviously increases the excitonic stability and slightly lowers the maximum points. The decrease in barrier width increases the stability, and may weaken the quantum confinement effect of a QW.

Acknowledgments

This work was supported by the National Natural Science Foundation of PR China (project 60566002), Specialized Research Fund for the Doctoral Program of Higher Education (project 20070126001) and project for excellent subject-directors of Inner Mongolia Autonomous Region.

References

[1] Akita K, Kyono T, Yoshizumi Y, Kitabayashi H and Katayama K 2007 *J. Appl. Phys.* **101** 033104

[2] Swietlik T, Franssen G, Czernecki R, Leszczynski M, Skierbiszewski C, Grzegory I, Suski T and Perlin P 2007 *J. Appl. Phys.* **101** 083109

[3] Asif Khan M, Shatalov M, Maruska H P, Wang H M and Kuokstis E 2005 *Japan. J. Appl. Phys.* **44** 7191

[4] Pokatilov E P, Nika D L and Balandin A A 2006 *Appl. Phys. Lett.* **89** 113508

[5] Tchernycheva M, Nevou L, Doyennette L, Julien F H, Warde E, Guillot F, Monroy E, Bellet-Amalric E, Remmele T and Albrecht M 2006 *Phys. Rev.* B **73** 125347

[6] Wagner J-M and Bechstedt F 2000 *Phys. Rev.* B **62** 4526

[7] Gõni A R, Siegle H, Syassen K, Thomsen C and Wagner J-M 2001 *Phys. Rev.* B **64** 035205

[8] Łepkowski S P, Teisseyre H, Suski T, Perlin P, Grandjean N and Massies J 2001 *Appl. Phys. Lett.* **79** 1483

[9] Vaschenko G, Patel D, Menoni C S, Gardner N F, Sun J, Götz W, Tomé C N and Clausen B 2001 *Phys. Rev.* B **64** 241308

[10] Ban S L and Liang X X 2001 *J. Lumin.* **94/95** 417

[11] Zhao G J, Liang X X and Ban S L 2003 *Mod. Phys. Lett.* B **17** 863

[12] Zhao G J, Liang X X and Ban S L 2003 *Phys. Lett.* A **319** 191

[13] Bigenwald P, Kavokin A, Gil B and Lefebvre P 2000 *Phys. Rev.* B **61** 15621

[14] Bigenwald P, Kavokin A, Gil B and Lefebvre P 2001 *Phys. Rev.* B **63** 035315

[15] Kalliakos S, Lefebvre P and Taliercio T 2003 *Phys. Rev.* B **67** 205307

[16] Nardelli M B, Rapcewicz K and Bernholc J 1997 *Phys. Rev.* B **55** R7323

[17] Shan W, Hauenstein R J, Fischer A J, Song J J, Perry W G, Bremser M D, Davis R F and Goldenberg B 1996 *Phys. Rev.* B **54** 13460

[18] Adachi S 1985 *J. Appl. Phys.* **58** R1

[19] Ban S L and Hasbun J E 1999 *Eur. Phys. J.* B **8** 453

[20] Tuchman J A and Herman I P 1992 *Phys. Rev.* B **45** 11929

[21] Perlin P, Mattos L, Shapiro N A, Kruger J, Wong W S, Sands T, Cheung N W and Weber E R 1999 *J. Appl. Phys.* **85** 2385

[22] Wagner J-M and Bechstedt F 2002 *Phys. Rev.* B **66** 115202

[23] Ting D Z-Y and Chang Y-C 1987 *Phys. Rev.* B **36** 4359

[24] Bernardini F, Fiorentini V and Vanderbilt D 1997 *Phys. Rev.* B **56** R10024

[25] Gõni A R, Syassen K and Cardona M 1990 *Phys. Rev.* B **41** 10104

[26] Pikus F G 1992 *Sov. Phys.—Semicond.* **26** 26

[27] Hasbun J E and Nee T W 1991 *Phys. Rev.* B **44** 3125

[28] Park S-H and Chuang S-L 2000 *J. Appl. Phys.* **87** 353

[29] Vurgaftman I, Meyer J R and Ram-Mohan L R 2001 *J. Appl. Phys.* **89** 5815

[30] Wei S H and Zunger A 1991 *Phys. Rev.* B **60** 5404

[31] Lambrecht W R L, Kim K, Rashkeev S N and Segall B 1996 *Mater. Res. Soc. Symp. Proc.* **395** 455

[32] Majewski J A, Stadele M and Vogl P 1997 *Mater. Res. Soc. Symp. Proc.* **449** 887

[33] Phillips J C 1973 *Bonds and Bands in Semiconductors* (San Diego, CA: Academic)

[34] Kleinman D A 1985 *Phys. Rev.* B **32** 3766