Binding Energies of Screened Excitons in a Strained (111)-Oriented Zinc-Blende GaN/AlGaN Quantum Well Under Hydrostatic Pressure*

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Abstract: We investigate the binding energies of excitons in a strained (111)-oriented zinc-blende GaN/$Al_{0.3}Ga_{0.7}N$ quantum well screened by the electron-hole (e-h) gas under hydrostatic pressure by combining a variational method and a self-consistent procedure. A built-in electric field produced by the strain-induced piezoelectric polarization is considered in our calculations. The result indicates that the binding energies of excitons increase nearly linearly with pressure, even though the modification of strain with hydrostatic pressure is considered, and the influence of pressure is more apparent under higher e-h densities. It is also found that as the density of an e-h gas increases, the binding energies first increase slowly to a maximum and then decrease rapidly when the e-h density is larger than about $1\times10^{11}cm^{-2}$. The excitonic binding energies increase obviously as the barrier thickness decreases due to the decrease of the built-in electric field.

Key words: exciton; strained zinc-blende quantum well; pressure; screened effect

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1 Introduction

In recent years, the group-Ⅲ nitride semiconductors have shown promise for application in devices, such as light emitting diodes (LEDs) and laser diodes (LDs)[1~3]. Such materials can be grown either in wurtzite or zinc-blende crystalline forms. Although the natural polytype of the materials is wurtzite, the zinc-blende structure was studied extensively in the last few years[4~6] and has been proved to be epitaxially stable. In particular, the piezoelectric charges induced by lattice-mismatch present at the interfaces and induce a large built-in electric field to influence the excitons in the quantum well (QW) consisting of group-Ⅲ nitride materials.

In the last decade, the pressure behavior of physical parameters, such as effective masses, energy gaps and phonon modes were investigated in succession. Wagner and Bechstedt[7] presented the *ab initio* calculations of the structural, dielectric, and lattice-dynamical properties of the zinc-blende and wurtzite GaN and AlN under hydrostatic pressure. Goñi *et al*.[8] investigated the pressure behavior of phonon modes on the hexagonal (wurtzite) and cubic (zinc-blende) modifications of GaN and hexagonal AlN experimentally. Considering the built-in electric field in the group-Ⅲ nitride heterostructures, Łepkowski *et al*.[9] investigated the behavior of light emission under hydrostatic pressure. A linear increase of the field was found when the pressure increased.

Using a variational method, Ban *et al*. calculated the binding energies of donors[10] under pressure in a realistic GaAs/$Al_xGa_{1-x}As$ heterojunction and excitons[11] in GaAs/AlAs QWs. Furthermore, the binding energies of donors versus pressure in GaAs/Al_xGa_{1-x}-As and no-strained zinc-blende GaN/$Al_xGa_{1-x}N$ QWs were calculated[12], respectively. The results indicated that the binding energies for both of the donor and exciton increase nearly linearly with the pressure. On the other hand, Bigenwald *et al*.[13,14] calculated the exciton states with a self-consistent procedure by solving both the Schrödinger and Poisson equations for electron and hole wave functions, and obtained peculiar, non-monotonic behavior of the exciton binding energy as a function of the e-h density.

However, the screening influence, due to the free two-dimensional e-h gas, on the binding energies of excitons in strained (111)-oriented zinc-blende QWs under hydrostatic pressure has not been investigated. This gap motivates us to investigate the pressure coefficients on the strained QW and then calculate the binding energies of the excitons confined in such a system. In this work, we shall restrict ourselves to the polarization along the (111)-oriented axis, which is along the growth direction of the GaN/$Al_xGa_{1-x}N$ QW. The result shows that the binding energies of ex-

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citons are rapidly decreased by the e-h gas with a high density about 1×10^{11} cm^{-2}, and nearly linearly increased by the hydrostatic pressure. Moreover, the built-in electric field in a QW with infinitely thick barriers is larger than that with finitely thick barriers and induces smaller excitonic binding energies in the former than that in the latter.

2 Model and calculation

In this work, we consider a strained (111)-oriented zinc-blende GaN/$Al_{0.3}Ga_{0.7}N$ QW with finite height barriers under the influence of e-h gas to calculate the binding energies of excitons as functions of the e-h density under hydrostatic pressure. Moreover, the built-in electric field induced in the biaxially and uniaxially strained QW is considered.

Without losing 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. The motion of carriers in the z direction is quantized and can be separated from the plane wave in the x-y direction. A self-consistent procedure by solving both the Schrödinger and Poisson equations is adopted to determine the ground state for electrons (holes) in a QW.

The Schrödinger equation for an electron (hole) in the z direction can be written as

$$\left\{-\frac{\hbar^2}{2}\times\frac{\partial}{\partial z}\left[\frac{1}{m_j^{\perp}(z)}\times\frac{\partial}{\partial z}\right]+V_j(z)+q_j[F(z)+\varphi_j(z)]z\right\}\Psi_j(z)=E_j\Psi_j(z) \quad (1)$$

where the superscript j = e, h denotes the electron and hole, respectively. $V_j(z)$ is the corresponding band offset for the QW. The ratio of the conduction and valence band offsets is 6:4 and assumed to be invariant with the pressure. The charge q_j is e for an electron and $-$e for a hole, respectively.

The strain-dependent energy gaps[15] of zinc-blende GaN and AlN material are

$$E_{g,w}=E_{g,w}(0)+(a_w^c-a_w^v)(2\varepsilon_{xx,w}+\varepsilon_{zz,w}) \quad (2)$$

and
$$E_{g,b(AlN)}=E_{g,b(AlN)}(0)+(a_b^c-a_b^v)(2\varepsilon_{xx,b}+\varepsilon_{zz,b}) \quad (3)$$

where a_i^c and a_i^v (i = w, b donates the well and barrier material, respectively) are the deformation potentials of conduction and valence band, respectively. The energy gap of $Al_xGa_{1-x}N$, which is chosen to be the barrier, can be calculated with the simplified coherent potential approximation[16] as

$$E_{g,b}=\frac{E_{g,w}E_{g,b(AlN)}}{xE_{g,w}+(1-x)E_{g,b(AlN)}} \quad (4)$$

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

$$\varepsilon_{xx,w}=\varepsilon_{yy,w}=\varepsilon_{/\!/,w}^{c}=\frac{a_b(p)-a_w(p)}{a_w(p)} \quad (5)$$

and

$$\varepsilon_{xx,b}=\varepsilon_{yy,b}=\varepsilon_{/\!/,b}^{c}=\frac{a_w(p)-a_b(p)}{a_b(p)} \quad (6)$$

where the lattice constant dependence of the hydrostatic pressure[17] is

$$a_i(p)=a_i(0)\left(1-\frac{p}{3B_{0,i}}\right) \quad (7)$$

with $B_{0,i}$ as the bulk modulus.

The uniaxial and biaxial strain tensor ratio can be expressed by[18]

$$\varepsilon_{zz,i}=-\frac{\varepsilon_{/\!/,i}^{c}}{\sigma^{(111)}} \quad (8)$$

where

$$\sigma^{(111)}=\frac{C_{11}^c+2C_{12}^c+4C_{44}^c}{2C_{11}^c+4C_{12}^c-4C_{44}^c} \quad (9)$$

Furthermore, the dependence of the energy gaps on hydrostatic pressure is considered by the following expression[19]:

$$E_{g,i}(p)=E_{g,i}+\alpha_i p \quad (10)$$

Then, the hydrostatic-pressure-modified biaxial and uniaxial strain dependence of the energy gaps is fully considered by inserting Eqs. (2)～(4) into Eq. (10).

Following the energy gaps given above, the biaxial, uniaxial, and hydrostatic pressure dependences of the effective masses[20] of electrons can be given by

$$\frac{m_0}{m_{e,i}^{\perp,/\!/}(p)}=1+\frac{C}{E_{g,i}(p)} \quad (11)$$

In Eq. (1), the internal electric field $F(z)$ is different in the well and barriers. Spontaneous polarization is absent in the zinc-blende crystals, but the piezoelectric polarization must be considered to calculate the built-in electric field[21] in the well and barriers with

$$F_w=\frac{L_b(P_b^{pz}-P_w^{pz})}{L_b\kappa_{0w}+L_w\kappa_{0b}} \quad (12)$$

and

$$F_b=\frac{L_w(P_w^{pz}-P_b^{pz})}{L_b\kappa_{0w}+L_w\kappa_{0b}} \quad (13)$$

respectively. Here the strain-induced piezoelectric polarizations can be written as

$$P_i^{pz}=2e_{14,i}\varepsilon'_{mn,i} \quad (14)$$

where $e_{14,i}$ is the piezoelectric constant, and $\varepsilon'_{mn,i}$ is the symmetrized strain component[22],

$$\varepsilon'_{xx,i}=\varepsilon'_{yy,i}=\varepsilon'_{zz,i}=\frac{1}{3}\times\left(2-\frac{1}{\sigma^{(111)}}\right)\varepsilon_{/\!/,i}^{c} \quad (15)$$

$$\varepsilon'_{xy,i}=\varepsilon'_{yz,i}=\varepsilon'_{zx,i}=-\frac{1}{3}\times\left(1+\frac{1}{\sigma^{(111)}}\right)\varepsilon_{/\!/,i}^{c} \quad (16)$$

If the barriers are infinitely wide, then the built-in electric field in the barriers will vanish, whereas F_w can be obtained by Eq. (12) with the limit of $L_b\to\infty$.

In Eq. (1), $\varphi_j(z)$ is the field obtained by solving the Poisson equation:

$$\frac{\partial\varphi_j(z)}{\partial z}=\frac{q_jN_sf(z)}{\kappa_0(z)} \quad (17)$$

where $f(z)=\Psi_e^2(z)-\Psi_h^2(z)$. $\kappa_0(z)$ is the material-

Table 1 Physical parameters of zinc-blende GaN and AlN The lattice constants are in units of angstrom, energy gaps, and deformation potentials in eV, the elastic constants in GPa, piezoelectric constants in C/m^2, and phonon frequencies in cm^{-1}.

	a	E_g	a^c	a^v	C_{11}	C_{12}	C_{44}	e_{14}	κ_∞	ω_{LO}	ω_{TO}	γ_{LO}	γ_{TO}
GaN	4.50[a]	3.3[a]	−2.2[a]	−5.2[a]	293[a]	159[a]	155[a]	−1.110[b]	5.41[c]	731[e]	551[e]	1.02[f]	1.19[f]
AlN	4.38[a]	4.9[a]	−6.0[a]	−3.4[a]	304[a]	160[a]	193[a]	−0.526[b]	4.46[d]	908[e]	654[e]	0.89[f]	1.14[f]

[a] Ref.[25] [b] Ref.[22] [c] Ref.[26]
[d] Ref.[27] [e] Ref.[28] [f] Ref.[7]

dependent static dielectric constant, and N_s is the e-h density. Then, the single particle (electron or hole) energy level E_j and wave function $\Psi_j(z)$ can be obtained by solving Eqs.(1) and (17) self-consistently.

The Hamiltonian of the e-h coupling can be written as

$$H_{e-h} = -\frac{\hbar^2}{2\mu_{e-h}} \times \frac{1}{\rho} \times \frac{\partial}{\partial \rho}\left(\rho \frac{\partial}{\partial \rho}\right) + e\varphi_{e-h}(z_e, z_h, \rho) \tag{18}$$

where ρ is the distance between the electron and hole in the x-y plane, and $\mu_{e-h} = m_e^{/\!/} m_h^{/\!/} / (m_e^{/\!/} + m_h^{/\!/})$ is the reduced mass of the exciton, in which $m_e^{/\!/}$ and $m_h^{/\!/}$ are the effective masses of the electron and hole parallel to the x-y plane, respectively.

The screened coulombic potential[13,14] of excitons is given in the representation of resultant mixed (z, q) as

$$e\varphi_{e-h}(z_e, z_h, q) = \frac{e^2}{4\pi\kappa_0 q}\left\{ e^{-q|z_e - z_h|} - \frac{\left[\int du e^{-q|u - z_e + z_h|} f(u)\right]^2}{\frac{q}{q_s} + \int du f(u) \int du' f(u') e^{-q|u-u'|}} \right\} \tag{19}$$

where $q_s = 2\mu e^2 / 4\pi\kappa_0 \hbar^2$ is the reciprocal screening radius. A variational method will be used below to calculate the variational energy of excitons in the x-y plane.

In Eqs.(12), (13), (17) and (19), the dielectric constants are influenced by the biaxial, uniaxial strains, and hydrostatic pressure, respectively. The static dielectric constant κ_0 of zinc-blende structure can be derived from the generalized Lyddane-Sachs-Teller relation

$$\kappa_0 = \kappa_\infty \left(\frac{\omega_{LO}}{\omega_{TO}}\right)^2 \tag{20}$$

where the hydrostatic pressure dependence of LO- and TO-phonon frequencies $\omega_{j,\alpha\alpha}$ can be determined by the given mode-Grüneisen parameter

$$\gamma_j = B_0 \frac{1}{\omega_j} \times \frac{\partial \omega_j(p)}{\partial p} \tag{21}$$

The dependence of the hydrostatic pressure on the phonons with a high frequency is given in Ref.[23], and can be rewritten as

$$\frac{\partial \kappa_\infty(p)}{\partial p} = -\frac{5(\kappa_\infty - 1)}{3B_0} \times (0.9 - f_i) \tag{22}$$

where f_i is the ionicity of the material.

A one-parameter trial wave function in the x-y plane for an exciton is given by Pikus[24]:

$$\Psi(\rho) = A e^{-\beta\rho} \cos(k_F \rho) \tag{23}$$

The variational energy of an exciton at ground state can be written as:

$$E_{e-h} = \langle \Psi | H_{e-h} | \Psi \rangle = \int dz_e |\Psi(z_e)|^2 \int dz_h |\Psi(z_h)|^2 \int d^2\rho \Psi^*(\rho) H_{e-h} \Psi(\rho) \tag{24}$$

Then, the total confined energy is given by:

$$E(\beta) = \sum_{i=e,h} E_i + E_{e-h} \tag{25}$$

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

$$E_b = E_{free} - E \tag{26}$$

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 derived by repeating the above process but neglecting the coulombic potential in Eq.(18) and replacing Eq.(23) by $\Psi(\rho_j) = e^{i k_F \cdot \rho_j} / 2\pi$ for the electron and hole.

3 Results and discussion

The parameters used in our computation are listed in Table 1. The calculated results are shown in Figs.1～4, respectively.

Figure 1 shows that the built-in electric field increases with hydrostatic pressure for QWs with infinitely and finitely thick barriers. When the barrier thickness is set equal to the well (5nm), the fields in the well and barriers are equal, but in opposite direc-

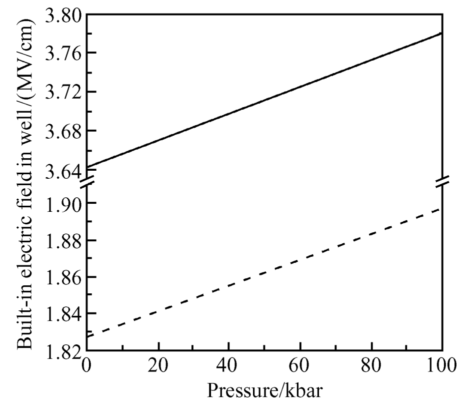

Fig.1 Built-in electric fields as functions of the hydrostatic pressure in QWs with infinite (solid line) and finite (dashed line) thick barriers, respectively

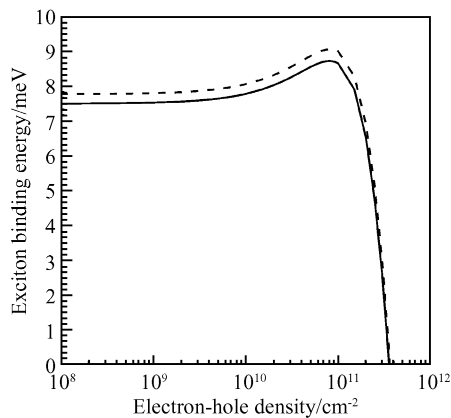

Fig. 2 Binding energies of excitons screened by the e-h gas in the strained zinc-blende $GaN/Al_{0.3}Ga_{0.7}N$ QW with infinite (solid line) and finite (dashed line) thick barriers as functions of the e-h density under 0kbar pressure, respectively

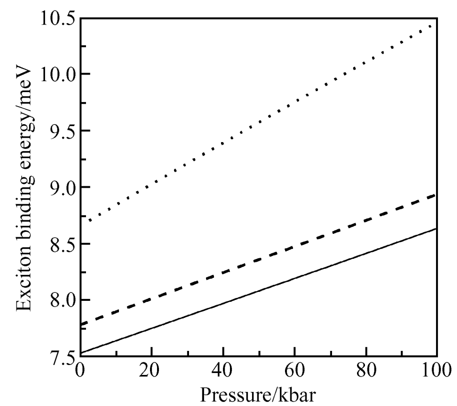

Fig. 4 Binding energies of excitons in a strained zinc-blende $GaN/Al_{0.3}Ga_{0.7}N$ QW with infinitely thick barriers as functions of pressure in the e-h densities equal to $1\times10^{9}\,cm^{-2}$ (solid line), $1\times10^{10}\,cm^{-2}$ (dashed line) and $1\times10^{11}\,cm^{-2}$ (doted line), respectively

tions. When the barrier is assumed to be infinitely thick, the built-in electric field in the barriers vanishes. Moreover, the absolute value of the built-in electric field increases 3.79% and 3.83% as the pressure increases from 0 to 100 kbar in QWs with infinitely and finitely thick barriers, respectively.

Figure 2 shows the binding energies of excitons screened by the e-h gas in a strained zinc-blende (111)-oriented QW with infinitely and finitely thick barriers as functions of the e-h density, respectively. The results indicate that the binding energies of excitons in both cases first increase slowly to a maximum as the density of the e-h gas increases, and then decrease rapidly when the density is larger than about $1\times10^{11}\,cm^{-2}$. When the barriers are finite and set equal to the well thickness (5nm), the built-in electric fields in the well and barriers are both 1.83MV/cm, but in the opposite direction, under zero hydrostatic pressure. However, when the barrier is assumed to be infinite, the built-in electric field vanishes and the

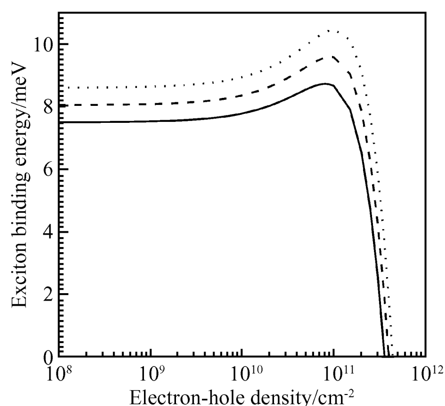

Fig. 3 Binding energies of excitons in a strained zinc-blende $GaN/Al_{0.3}Ga_{0.7}N$ QW with infinite thick barriers as functions of the e-h densities under pressure of 0 (solid line), 50 (dashed line) and 100kbar (dotted line), respectively

field in the well is twice as much as the field with finite barrier thickness, and the binding energy decreases 3.49%.

Figure 3 shows the binding energies of excitons in a strained zinc-blende $GaN/Al_{0.3}Ga_{0.7}N$ QW calculated as functions of the e-h density under various pressures, where the thickness of the barriers is infinite. The changing tendency of the exciton binding energies with the e-h density in 50kbar and 100kbar is similar to that under zero pressure. Namely, as the e-h density increases, the binding energies first increase slowly to a maximum because of the screening of the built-in electric field, and then decrease rapidly in high density about $1\times10^{11}\,cm^{-2}$ because of the huge increase in the kinetic energy of the e-h relative motion due to the exclusion effect[14,24].

Figure 4 shows the binding energies of excitons in a strained zinc-blende $GaN/Al_{0.3}Ga_{0.7}N$ QW with an infinitely thick barrier calculated as functions of pressure in different e-h densities. The results indicate that the binding energies of exciton increase nearly linearly as the pressure increases in various e-h densities. When the pressure increases from 0 to 100kbar, the percentages of the excitonic binding energies are increased by 14.74%, 14.91%, and 20.89% for the e-h densities equal to 1×10^{9}, 1×10^{10}, and $1\times10^{11}\,cm^{-2}$, respectively. This finding indicates that the influence of the pressure is more apparent under a higher e-h density.

4 Summary

In summary, the binding energies of excitons in a biaxially and uniaxially strained (111)-oriented zinc-blende $GaN/Al_{0.3}Ga_{0.7}N$ QW are calculated by considering both the hydrostatic pressure effect and

screening due to e-h gas. A variational method and a self-consistent procedure are combined to calculate the binding energy of the exciton influenced by the strain-induced piezoelectric polarization induced built-in electric field. The results indicate that the binding energies of excitons increase nearly linearly with pressure when the modification of strain with hydrostatic pressure is considered. The influence of the pressure is more apparent under a higher e-h density. We also found that as the e-h density increases, the binding energies first increase slowly to a maximum and then decrease rapidly when the e-h density is larger than about $1\times10^{11}\,cm^{-2}$, and as the barrier thickness decreases, the excitonic binding energies increase due to the decrease of the built-in electric field.

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流体静压力下应变闪锌矿(111)取向GaN/AlGaN量子阱中受屏蔽激子的结合能*

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摘要： 结合变分法与自洽计算方法研究了流体静压力下应变闪锌矿(111)取向GaN/$Al_xGa_{1-x}N$量子阱中受电子-空穴气体屏蔽的激子结合能.计算中，考虑了沿(111)取向生长多层结构时存在压电极化引起的内建电场.计算结果表明，考虑压力对双轴及单轴应变的调制以及禁带宽度、有效质量和介电常数等参数的压力效应时，激子结合能随压力的增大近似线性增加；且当电子-空穴气体密度大时，这一效应更加显著.当给定压力时，随着电子-空穴气面密度的增加，激子结合能先缓慢增加，但当密度达到大约$10^{11}cm^{-2}$时结合能开始迅速衰减.此外，当减小垒的厚度时，由于内建电场减弱，激子结合能显著增加.

关键词： 激子；应变闪锌矿量子阱；压力；屏蔽效应

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