Influence of pressure on donor bound exciton states in wurtzite InGaN/GaN quantum dot nanowire heterostructures

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The effects of hydrostatic pressure and strong built-in electric field on the donor bound exciton states confined in wurtzite $In_xGa_{1-x}N$/GaN strained quantum dot (QD) nanowire heterostructures (NWHETs) are investigated using a variational method under the effective mass and simplified coherent potential approximations. The results show that the hydrostatic pressure has a significant influence on the bound exciton states and interband optical transitions. The bound exciton binding energy almost linearly increases if the hydrostatic pressure increases. The emission wavelength has a blue-shift if the hydrostatic pressure increases and a red-shift if the QD height increases. The bound exciton binding energy more obviously depends on the hydrostatic pressure for the small radius or the large height QDs. The hydrostatic pressure can effectively enhance the exciton oscillator strength and improve the light emission efficiency of $In_xGa_{1-x}N$/GaN QD NWHETs.

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1. Introduction

The GaN-based nanoscale structures, such as the high-quality one-dimensional $In_xGa_{1-x}N$ nanowires (NWs) and $In_xGa_{1-x}N$/GaN quantum-dot (QD) NW heterostructures (NWHETs) have been successfully fabricated recently [1–3]. It has been well-accepted that the impurity plays an essential role in controlling physical properties of semiconductors, such as the optical, electrical and transport characteristics. Many theoretical works are focused on the donor bound excitons and related issues [4,5]. The high pressure, as a powerful tool, is quite useful for studying the electronic properties of semiconductors and determining the carrier recombination processes. The electronic and optical properties of III-V nitride compound semiconductors under pressure have been extensively studied by experiments and theories [6–10]. The donor bound excitons in a prolate ellipsoidal finite-potential QD under hydrostatic pressure have also been studied by using the perturbation theory [9].

To the best of our knowledge, the influence of the hydrostatic pressure on the bound exciton states and optical properties in wurtzite $In_xGa_{1-x}N$/GaN coupled QD NWHETs has not been studied in depth. We will thus pay our attention to the influence of the hydrostatic pressure on the confined donor exciton states in wurtzite $In_xGa_{1-x}N$ /GaN QD NWHETs. We find that the hydrostatic pressure, strong built-in electric field (BEF), impurity position and lattice mismatch have a significant influence on bound exciton states and interband optical transitions.

2. Model and theory

Considering the hydrostatic pressure effect, we investigate an donor bound exciton confined in a cylindrical wurtzite $In_xGa_{1-x}N$ strained coupled QDs with height H_D embedded in a [0001]-oriented (z-direction) GaN NW with radius R. Within the framework of the effective-mass approximation, the donor bound exciton Hamiltonian can be written as,

$$\hat{H}_{\mathbf{DX}} = \hat{H}_i - \frac{e^2}{4\pi\varepsilon^{(0)}\varepsilon_0}\left(\frac{1}{|\vec{r}_e - \vec{r}_i|} - \frac{1}{|\vec{r}_h - \vec{r}_i|} + \frac{1}{|\vec{r}_e - \vec{r}_h|}\right), \quad (1)$$

where $\vec{r}_e$, $\vec{r}_h$ and $\vec{r}_i$ denote the position vector of the electron, hole and impurity, respectively. The $\varepsilon^{(0)}$ is the static dielectric constant of the $In_xGa_{1-x}N$ QD. The Hamiltonian $\hat{H}_i$ of the electron (hole) confined in the cylindrical $In_xGa_{1-x}N$ QD is given by,

$$\hat{H}_i = -\frac{\hbar^2}{2}\left\{\frac{1}{m_{\perp i}}\left[\frac{1}{\rho_i}\frac{\partial}{\partial\rho_i}\left(\rho_i\frac{\partial}{\partial\rho_i}\right)+\frac{1}{\rho_i^2}\frac{\partial^2}{\partial\theta_i^2}\right]+\frac{1}{m_{zi}}\frac{\partial^2}{\partial z_i^2}\right\}+V(\rho_i,z_i)\mp eFz_i \cdot \quad (2)$$

Where m_{zi} and $m_{\perp i}$ are the effective mass of the electron (hole) along and perpendicular to the [0001]-direction, and $V(\rho_i,z_i)$ is the electron (hole) confinement potential.

Quantities of interest include the donor exciton binding energy E_b, closely related to the strength of the Coulomb interaction between the electron and hole, the impurity and electron, as well as the impurity and hole. The exciton oscillator strength f_{ex}, which determines the radiative lifetime of the donor bound excitons and sensitively depends on the confinement of the electron and hole wavefunctions and the overlap between them. Generally, E_b can be computed as follows:

$$E_b = E_e + E_h - E_{\mathrm{DX}} \quad (3)$$

where E_e (E_h) is the electron (hole) confinement energy and E_{DX} is the donor bound exciton energy defined as

$$E_{\mathbf{DX}} = \min_{\{\alpha,\beta\}} \frac{\left\langle \Phi(\vec{r}_e,\vec{r}_h)\left|\hat{H}_{\mathbf{DX}}\right|\Phi(\vec{r}_e,\vec{r}_h)\right\rangle}{\left\langle \Phi(\vec{r}_e,\vec{r}_h)\middle|\Phi(\vec{r}_e,\vec{r}_h)\right\rangle}. \quad (4)$$

Considering the correlation of the electron-hole relative motion, the trial wave function of the exciton confined in $In_xGa_{1-x}N$/GaN QD NWHETs can be chosen as the same form as in Ref.[11].

Using the envelope-function approximation, the oscillator strength for the exciton ground state is given as follows:

$$f_{ex} = \frac{2Q^2}{m_0(E_{\mathrm{DX}}-E_0)}\left|\int \Phi(\vec{r}_e,\vec{r}_h)d\vec{r}_e\right|^2 \quad (5)$$

where Q describes all intracell matrix-element effects, m_0 is the bare electron mass and E_0 is the energy of the state without the exciton. The oscillator strength f_{ex} not only defines the strength of absorption lines but also relates to the radiative decay time τ defined as

$$\tau = \frac{2\pi\varepsilon_0 m_0 c^3\hbar^2}{ne^2E_{ph}^2 f_{ex}}, \quad (6)$$

where E_{ph} is the photon energy, n is the refractive index of $In_xGa_{1-x}N$ ternary alloy, and $\varepsilon_0, m_0, c, \hbar$, and e are fundamental physical constants with their usual meaning.

In this paper, we considered the influence of the hydrostatic pressure. The material parameters, such as the components of uniaxial and biaxial strain tensors of material, the lattice constant, the pressure-dependent energy gaps, the electron and hole effective masses, the static dielectric constant, the piezoelectric polarization, the NW radius R and the QD height H_{D}, all depend on the hydrostatic pressure P. Pressure and strain dependence of physical parameters and the other material parameters are the same as in Ref.[12]

3. Numerical results and discussion

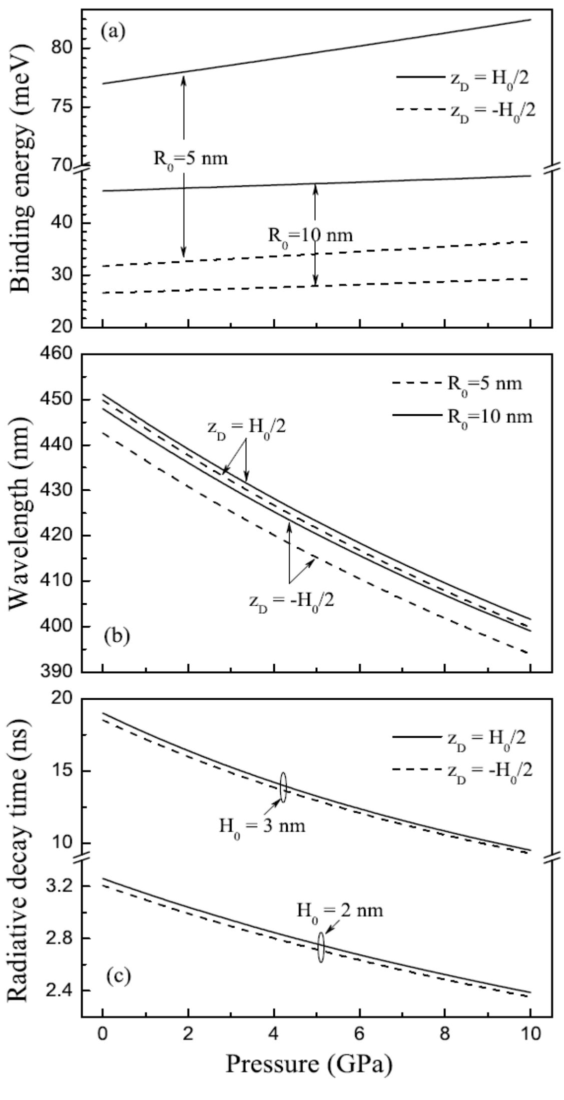

Fig. 1. The bound exciton binding energy (a), the emission wavelength (b) and the radiative decay time (c) as a function of the hydrostatic pressure P in cylindrical wurtzite $In_{0.2}Ga_{0.8}N$/GaN strained QD NWHETs. Here we choose the QD height H_0 = 2 nm in (a) and (b) and the QD radius R_0 = 5 nm in (c).

In Fig. 1, we present our results for the bound exciton binding energy E_b, the emission wavelength and the radiative decay time as a function of the hydrostatic pressure P in the cylindrical wurtzite $In_{0.2}Ga_{0.8}N$ /GaN strained QD NWHETs. We can see from Fig. 1(a) that E_b increases almost linearly with the hydrostatic pressure P. This is mainly because the size of $In_{0.2}Ga_{0.8}N$ QDs ($R(P)$ and $H(P)$) and the dielectric constant are reduced if P increases. As a result, the relative distance $\overline{\rho}_{eh}$ and $\overline{z}_{eh}$ between the electron and hole and relative distance $\overline{z}_i$ between the electron and the donor impurity confined in QDs are decreased. The Coulomb interactions of the electron-hole and the electron-impurity are thus increased. Fig. 1(a) also indicates that E_b for the R_0 = 5 nm QD is larger than that for the R_0 = 10 nm QD. This is due to the in-plane relative distance between the electron and impurity decreases when R_0 is small. Moreover, the results also show that the hydrostatic pressure plays an important role in the exciton binding energy, especially for the small radius QDs. For example, considering the BEF and the donor position z_D=H_0/2, the difference of E_b for the two cases of P = 0 and 10 GPa for the QDs with R_0 = 5 nm is of 5.46 meV (a relative difference of 7.09%). The corresponding difference is of 2.88 meV (6.24%) for the R_0 = 10 nm QD. Fig. 3.4(a) also shows that the donor position has a remarkable influence on the donor bound exciton binding energy due to the Coulomb interaction between the electron (hole) and impurity.

Moreover, we can see from Fig. 1(b) that the emission wavelength has an obvious blue-shift if the hydrostatic pressure P increases. The physical reason is because the QD height H and radius R are reduced when P increases. This directly leads to increasing of the confined energy of the electron and hole in QD NWHETs. The band gaps of GaN and $In_xGa_{1-x}N$ alloy also increase due to increasing of P. Both of them make the emission wavelength display an obvious blue-shift. For example, for R_0 = 10 nm case, the emission wavelength is λ = 451.14 (401.58) nm with the hydrostatic pressure P=0 (10) GPa. The difference (relative difference) is $\Delta\lambda$ = 49.56 nm (11.0%). The result is similar to the R_0 = 5 nm case.

The radiative decay time τ, as an important physical quantity, is inversely proportional to the exciton oscillator strength and the square of the optical transition energy. We can see from Fig. 1(c) that τ decreases with increasing of P. For example, with the donor position z_D=H_0/2 and quantum dot height H_0 = 3 nm, τ decreases 9.51 ns (a relative difference of 49.9%) for the QD with R_0=5 nm in the two cases of P=0 and 10 GPa. The physical reason is that the electron-hole spatial separation decreases with P increasing. Hence the overlap integral between the electron and hole wave functions and the exciton oscillator strength become large if P increases. At the same time, the optical transition energy is also increased with increasing of the hydrostatic pressure. Hence the radiative decay time is reduced if P increases due to the above two important effects.

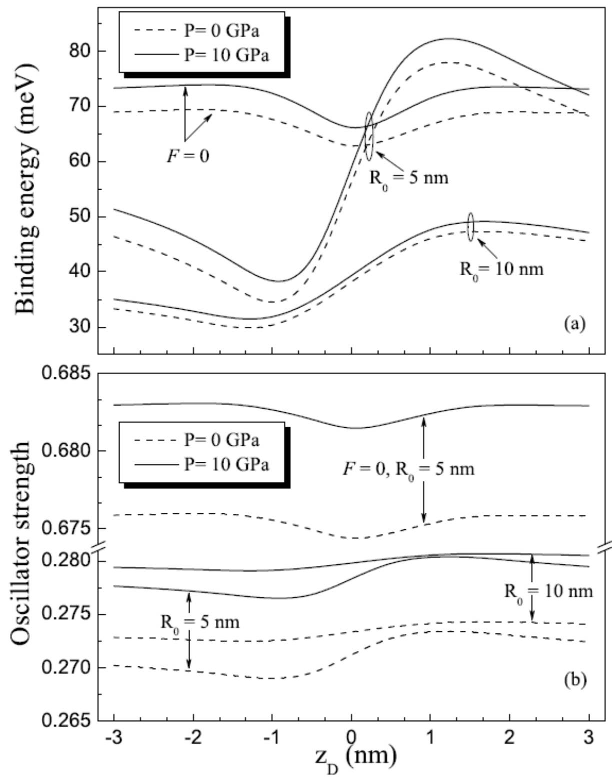

Fig. 2. The bound exciton binding energy (a) and the oscillator strength (b) as a function of the donor position z_D in cylindrical wurtzite $In_{0.2}Ga_{0.8}N$/GaN strained QD (H_0=2nm) NWHETs with different QD radius under hydrostatic pressures. For the sake of comparison, the bound exciton binding energy without the BEF (F = 0) has also been shown in (a).

Fig. 2 indicates that the donor bound exciton binding energy and the exciton oscillator strength *fex* as a function of the donor position with the different radius R in the cylindrical wurtzite $In_{0.2}Ga_{0.8}N$/GaN strained single-QD NWHETs. Fig. 2(a) clearly shows that both the donor position and the hydrostatic pressure have a significant influence on the donor bound exciton states. Moreover, we can see that the influence of the hydrostatic pressure on E_b for the donor position near the QD interface is larger than that for the donor position closing to the QD center. Furthermore, Fig. 2(a) also shows that the donor bound exciton binding energy without the BEF is symmetric about the QD center in the case of z_D=0. If fixing the donor position, E_b for the QD with small radius (R_0=5 nm) is larger than that for the large radius case (R_0=10 nm). This is because both the electron and hole are confined strongly in the small radius QD, which directly leads to the increment of the exciton binding energy.

In order to clarify the influences of the hydrostatic pressure, donor position and BEF on the oscillator strength, we calculated the exciton oscillator strength f_{ex} as a function of the donor position with the different radius R_0 with (without) the BEF in the cylindrical wurtzite

$In_{0.2}Ga_{0.8}N$ strained single-QD NWHETs in Fig. 2(b). We can see from Fig. 2(b) that the exciton oscillator strength is reduced if considering the BEF. This is because the electron-hole spatial separation in the *z*-direction becomes large due to the BEF. Fig. 2(b) also shows that the exciton oscillator strength slightly increases if the QD radius increases. The exciton oscillator strength insensitively depends on the donor position. The hydrostatic pressure plays an important role in f_{ex}. It can be clearly seen that the f_{ex} increases obviously with the increasing of P. The physical reason is that the electron-hole spatial separation decreases with P increasing. Hence the overlap integral between the electron and hole wave functions and the exciton oscillator strength become large if P increases.

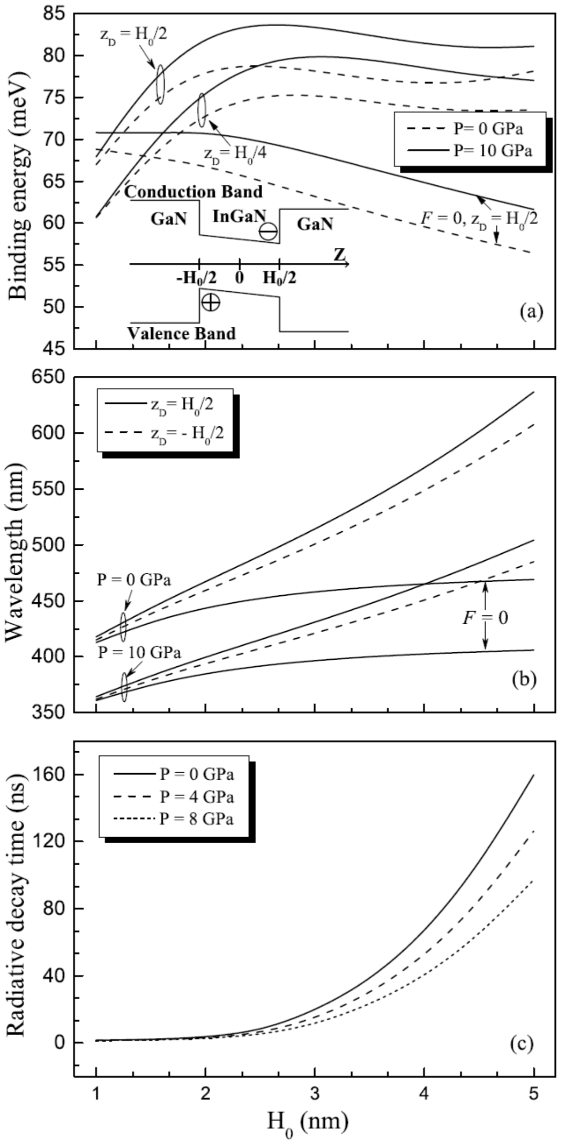

Fig. 3. The exciton binding energy (a), the emission wavelength (b) and the radiative decay time (c) as a function of the QD (R_0=5nm) height H_0 in cylindrical wurtzite $In_{0.2}Ga_{0.8}N/GaN$ strained QD NWHETs under different hydrostatic pressures.

Fig. 3 displays the exciton binding energy, emission wavelength and radiative decay time as a function of the QD height H_0, in which the hydrostatic pressure, strong BEF and different donor position effects are considered. Fig. 3(a) shows that the donor position has a remarkable influence on the donor bound exciton binding energy due to the Coulomb interaction between the electron (hole) and impurity. If the donor approaches the QD center, the donor bound exciton binding energy decreases obviously. This is because that the Coulomb repulsive interaction between the hole and the ionized positively charged donor becomes much larger than the Coulomb attractive interaction between the hole and the electron (see the inset of Fig.3 (a)). As a result, the donor binding energy decreases if the ionized donor is near the left-interface. The hydrostatic pressure plays a dominative role again, which leads to the increment of E_b.

Fig. 3 (b) shows that the emission wavelength λ monotonically increases if the QD height H_0 increases. For comparison, the emission wavelength without the BEF is also given. Furthermore, we can see from Fig. 3 (b) that the emission wavelength decreases when the pressure P increases. The influence of P on the emission wavelength becomes more obvious for the large height QDs. For instance, for the H_0=2nm and z_D=H_0/2 case, the net reduction of $\Delta\lambda$ is of 67.55 nm with percentage of 14.46% for the two cases of P=0 and 10 GPa. The corresponding difference is of 132.53 nm (20.81%) for the H_0=5nm case. This is because the physical parameters more sensitively depend on the pressure for the large height QDs. We also see that the influence of the BEF on the emission wavelength becomes more significant for the large height QDs than the small height QDs. Hence the strong BEF, the QD height and the pressure have a significant influence on the electron interband optical transitions.

In Fig. 3 (c), we further calculate the radiative decay time τ as a function of the QD height H_0 by considering the pressure and BEF effects. It can be seen that τ increases quickly if H_0 increases. The electron-hole separation in the z -direction becomes large when H_0 increases. This is the main reason which directly leads to a reduction of the exciton oscillator strength and optical transition energy. Hence the radiative decay time increases. Fig. 3.6(c) also demonstrates that the radiative decay time of the interband optical transition is large and increases almost two orders of magnitude from 1.53 ns for the H_0= 1 nm QD to 159.80 ns for the H_0=5 nm QD when P=0GPa. For the P=8GPa case, the corresponding radiative decay time increases from 1.35 ns for the H_0=1nm to 97.28 ns for the H_0=5nm. Hence the radiative decay time is reduced by the applied pressure, especially for the large QD height H_0.

We further investigate the donor bound exciton binding energy and the emission wavelength as a function of radius R0 in the cylindrical wurtzite $In_{0.2}Ga_{0.8}N/GaN$ strained single-QD NWHETs in Fig. 4. These data clearly indicate that the bound exciton binding energy decreases monotonically when R_0 increases. This is due to the increase of the electron-hole and electrondonor in-plane relative distance, which reduces the Coulomb interaction when R_0 increases. The hydrostatic pressure has a remarkable influence on the donor bound exciton states, especially for the small nanowire radius R_0. Fig. 4(b) indicates that the emission wavelength λ becomes insensitive to the NW radius if R_0>10 nm. The results of Fig. 4 clearly indicate that the pressure P and the radius R_0 have a remarkable influence on the donor bound exciton states and optical properties of $In_xGa_{1-x}N$ strained QD NWHETs.

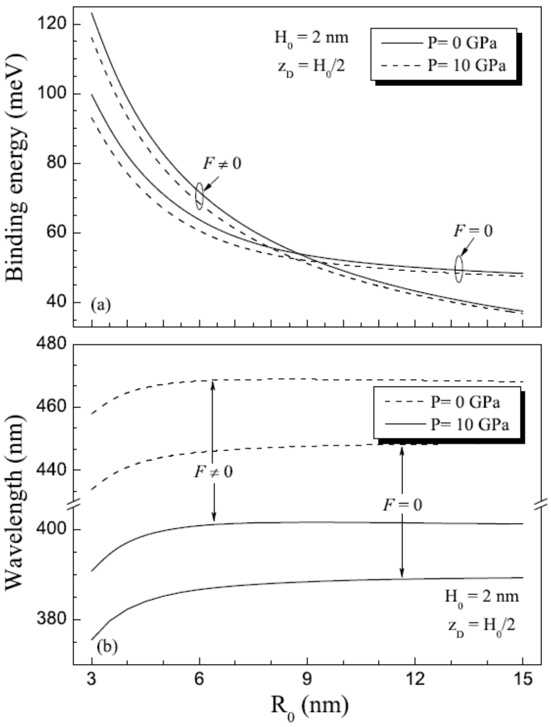

Fig. 4. The exciton binding energy (a) and the emission wavelength (b) as a function of the QD radius R_0 in cylindrical wurtzite $In_{0.2}Ga_{0.8}N$/GaN strained QD NWHETs under different hydrostatic pressures.

4. Conclusions

Considering the influence of the hydrostatic pressure, QD height and radius, donor position and strong BEF on the bound exciton binding energy, emission wavelength, oscillator strength and radiative decay time, we variationally calculate the bound exciton states confined in cylindrical wurtzite $In_xGa_{1-x}N$/GaN strained QD NWHETs in the framework of the effective mass and simplified coherent potential approximations. We found that the hydrostatic pressure and the QD structural parameters have a remarkable influence on donor bound exciton states. The bound exciton binding energy E_b increases almost linearly with the hydrostatic pressure P. The emission wavelength λ has a blue-shift if the hydrostatic pressure P increases. The radiative decay time is reduced if P increases. The donor bound exciton binding energy sensitively depends on the position of the ionized donor. The radiative decay time τ increases quickly if H0 increases and decreases if P increases, especially for the large QD height H0. The emission wavelength λ is insensitive to the NW radius if R_0 > 10 nm. The above results clearly indicate that the hydrostatic pressure has an important effect on the optical properties of the donor bound exciton states in wurtzite $In_xGa_{1-x}N$/GaN strained QD NWHETs. We hope that the present theory can stimulate further investigation of the physics as well as device applications based on the group-III nitride QD NWHETs.

Acknowledgments

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