Influence of strain on hydrogenic impurity states in a GaN/$Al_xGa_{1-x}N$ quantum dot*

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(Received 4 December 2008)

Within the effective-mass approximation, we calculated the influence of strain on the binding energy of a hydrogenic donor impurity by a variational approach in a cylindrical wurtzite GaN/$Al_xGa_{1-x}N$ strained quantum dot, including the strong built-in electric field effect due to the spontaneous and piezoelectric polarization. The results show that the binding energy of impurity decreases when the strain is considered. Then the built-in electric field becomes bigger with the Al content increasing and the binding energy of hydrogenic donor impurity decreases when the Al content is increasing. For dot height $L < 2$ nm, the change of the binding energy is very small with the Al content variety.

Document code: A **Article ID:** 1673-1905(2009)02-0085-4

DOI 10.1007/s11801-009-8161-4

In recent years, wide-band gap wurtzite (WZ) III-V nitrides semiconductors, such as InN, GaN, AlN and their ternary compounds have attracted more attention due to potential device applications. For example, they are widely used in the fabrication of optoelectronic devices: blue/ultraviolet lasers, laser diodes (LDs), light emitting diodes (LEDs), and ultraviolet detectors [1-3]. Moreover, the study of hydrogenic impurity is one of the main problems in semiconductor low dimensional systems because the presence of impurity in nanostructures influences greatly the electronic mobility and their optical properties. Since Bastard[4] worked on the donor binding energy of a hydrogenic impurity within an infinite potential well structure, the hydrogenic impurity states in semiconductor low dimensional systems have been widely studied in the last decades[5-11]. More recently, Mendoza et al.[12] investigated the stark effects on hydrogenic impurity in a cubic quantum dot. Movilla et al.[13] have dealt with dielectric mismatch effects on the donor binding energies in spherical quantum dot. The lower-lying states of the hydrogenic impurity in cylindrical quantum dot have been also investigated theoretically[14,15]. These studies show that the donor binding energy in nanoscopic systems depends upon materials, structure and impurity position.

The group-III nitrides are commonly produced in the WZ crystal structure with a strong spontaneous macroscopic polarization. Moreover, strains of the WZ GaN/AlGaN heterostructures, due to large lattice mismatch between GaN and AlGaN, can induce a remarkable piezoelectric polarization. This leads to a strong built-in electric field in order of MV/cm in the heterostructures. The electronic, dielectric and optical properties of the heterostructures are strongly affected by the built-in electric field. Lately, C.X. Xia and S.Y.Wei study variationally the binding energy of a hydrogenic donor impurity as functions of the impurity position and WZ InGaN strained quantum dot structural parameters. Al content of $Al_xGa_{1-x}N$ potential hill layer has close correlation with discontinuity and polarization effect of GaN/$Al_xGa_{1-x}N$ heterostructures interface conduction band. In this letter, we will study the influence of the Al content on the binding energy of a hydrogenic donor impurity by means of variational approach in GaN/$Al_xGaN_{1-x}N$ quantum dot.

According to previous theoretical studies on WZ GaN/$Al_xGaN_{1-x}N$ strained quantum dot, we consider an isolated cylindrical WZ $Al_xGa_{1-x}N$/GaN/$Al_xGa_{1-x}N$ strained quantum dot with radius R and height L, ignoring the strain effect of $Al_xGa_{1-x}N$ potential barrier layer.

Within the framework of effective-mass approximation, the Hamiltonian for a hydrogenic donor impurity in the cylindrical WZ GaN/$Al_xGaN_{1-x}N$ strained quantum dot may be written as,

$$\hat{H} = \hat{H}_0 - \frac{e^2}{4\pi\varepsilon_0\bar{\varepsilon}r} \quad , \tag{1}$$

* This work has been supported by the National Natural Science Foundation of China (No. 10564003) and the Key Project of the Science and Technology Research of the Educational Ministry of China (No. 208025)

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with

$$\hat{H}_0 = -\frac{\hbar^2}{2m^*}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}+\frac{\partial^2}{\partial z^2}\right]+V(\rho,z)+eFz\,, \tag{2}$$

where $r=\sqrt{(x-x_i)^2+(y-y_i)^2+(z-z_i)^2}$ is the distance between the electron and the impurity site, $x(x_i)$, $y(y_i)$ and $z(z_i)$ are the coordinates of the electron (impurity) in the quantum dot, e is the absolute value of the electron charge, ε_0 is the permittivity of the free space, and $\overline{\varepsilon}$ is the effective mean relative dielectric constant of the embedding material, m^* is the electron effective mass. The confining potential has the form as:

$$V(\rho,z)=\begin{cases}0, & \rho<R,|z|<L/2,\\ \infty, & \rho\geq R,|z|\geq L/2,\end{cases} \tag{3}$$

where R and L are the cylindrical dot radius and length, respectively.

The strength of the built-in electric field F caused by spontaneous and piezoelectric polarization in the WZ GaN/$Al_xGa_{1-x}N$ strained quantum dot is expressed as[16]

$$F=\begin{cases}\left|-\dfrac{P_{SP}^{GaN}+P_{PE}^{GaN}-P_{SP}^{Al_xGa_{1-x}N}}{\varepsilon_e^{GaN}\varepsilon_0}\right|, & |z|<L/2,\\ 0, & |z|\geqslant L/2,\end{cases} \tag{4}$$

where P_{SP}^{GaN}, P_{PE}^{GaN} and $P_{SP}^{Al_xGa_{1-x}N}$ are the spontaneous and piezoelectric polarization of GaN and the spontaneous polarization of $Al_xGa_{1-x}N$, respectively. ε_e^{GaN} is the electronic dielectric constant of material GaN. In general, the direction of the built-in electric field F depends on the orientation of the spontaneous and piezoelectric polarizations and it can be determined by both the polarity of the crystal and the strain of the quantum well (QW) structure [16]. Based on Eq. (4), we have calculated the strength of the built-in electric field F in the strained GaN layer as a function of the Al content x for the $Al_xGa_{1-x}N$/GaN/$Al_xGa_{1-x}N$ quantum dot. The result shows that the built-in electric field in the strained GaN layer is extremely strong, and it is of the order of MV/cm and becomes higher with the Al content increasing.

In order to calculate the ground-state energy of the hydrogenic impurity in a quantum dot, the trial wave function may be written as,

$$\Psi = \varphi(\rho,z)e^{-\alpha\rho_{ei}^2}e^{-\gamma z_{ei}^2}, \tag{5}$$

where $\varphi(\rho,z)$ is the eigenfunction of the Hamiltonian described in Eq. (2). If we assume that the in-plane and on-axis motions of the electron are weakly coupled, as has been done in an isolated cylindrical WZ GaN strained quantum dot, the wave function $\varphi(\rho,z)$ can be written as

$$\varphi(\rho,z)=\begin{cases}J_0(\kappa_{10}\rho/R)e^{-\beta z/L}, & \rho<R,|z|<L/2,\\ 0, & \rho\geq R,|z|\geq L/2,\end{cases} \tag{6}$$

where $J_0(\kappa_{10}\rho/R)$ is the ordinary Bessel function of order zero, the exponential term in Eq.(5) accounts for the presence of the hydrogenic impurity, α, β and γ are variational parameters. $\rho_{ei}^2=(x-x_i)^2+(y-y_i)^2$ and $z_{ei}^2=(z-z_i)^2$, we make $x_i=0$ and $y_i=0$ for sample.

The energy of the hydrogenic impurity in the WZ GaN/$Al_xGaN_{1-x}N$ strained quantum dot may be obtained by minimizing

$$E=\min_{\alpha,\gamma}\frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle}\,. \tag{7}$$

The donor binding energy E_b of the hydrogenic impurity can be given as follow

$$E_b = E_0 - E, \tag{8}$$

where E_b is the ground-state energy for the Hamiltonian of Eq. (2).

We have calculated the ground-state donor binding energy E_b as a function of Al content and the quantum dot structural parameters, such as dot height L and radius R for different impurity position. Furthermore, the effect of the strong built-in electric field due to spontaneous and piezoelectric polarizations is included. Material parameters used in the present article are the same as in Ref. [16].

Fig.1 shows the ground-state donor binding energy E_b of the on-center hydrogenic impurity as a function of radius of the GaN/$Al_{0.15}Ga_{0.85}N$ quantum dot, with the built-in electric field and without the built-in electric field. As expected, the ground-state donor binding energy decreases with the increase of the quantum dot radius considering the built-in electric field and ignoring the built-in electric field, due to the decrease of the electron quantum confinement. Fig.1 also shows that the ground-state donor binding energy with the built-in electric field is smaller than that without the built-in electric field for the same quantum dot radius. The reason is that the

built-in electric field moves the electron and impurity to reverse direction in quantum dot.

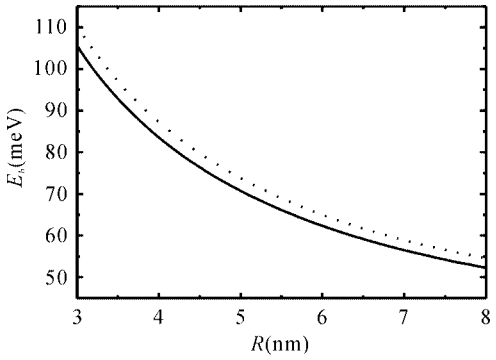
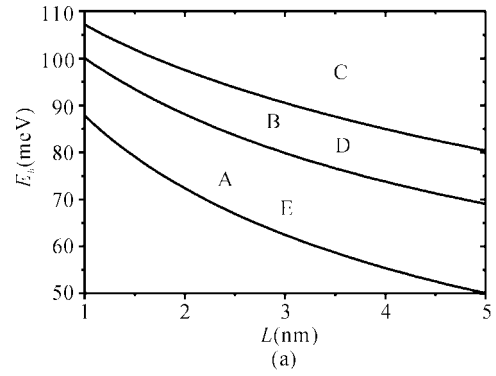


Fig.1 The ground-state donor binding energy E_b as a function of the radius R of the GaN/$Al_{0.15}Ga_{0.85}N$ quantum dot with L = 4 nm and z_i =0. The solid (dotted) line is with (without) the built-in electric field.

In Fig.2, we display the ground-state donor binding energy E_b as a function of the height L of the GaN/$Al_{0.15}Ga_{0.85}N$ strained quantum dot for different impurity position z_i with (without) the built-in electric field. Fig.2(a) shows that the donor binding energy curves A and E (B and D) are identical. Also, we can notice that the donor binding energy E_b for z_i = 0 (curve C) is larger than that for $z_i = \pm L/2$ (curve A or E) and $\pm L/4$ (curve B or D). The explanation is that the electron probability distribution is symmetric around $z_i = 0$ when the built-in electric field is ignored. Fig.2(a) also displays that the E_b decreases with the increase of the quantum dot height L. It can be explained that the average distance $\overline{z}_{ei}$ between the electron and the impurity is increased when L is increased. However, it can be seen that the E_b along curves A and E (B and D) are split because of the built-in electric field in Fig.2(b). Compared with Fig.2(a), it is indicated that the built-in electric field induces only small difference of the E_b when dot height L is relative small. The splitting increases when the dot height L increases. This result can be explained that the symmetrical break of the electron probability distribution around $z_i = 0$ increases the split due to the effect of the built-in electric field. From Fig.2(b), we also see that the E_b is decreased monotonically when the dot height L is increased for curves A, B, C, D and E, respectively. This is because the distance $\overline{z}_{ei}$ between the electron and the impurity is increased monotonically, the Coulomb interaction is reduced and the donor binding energy decreases.



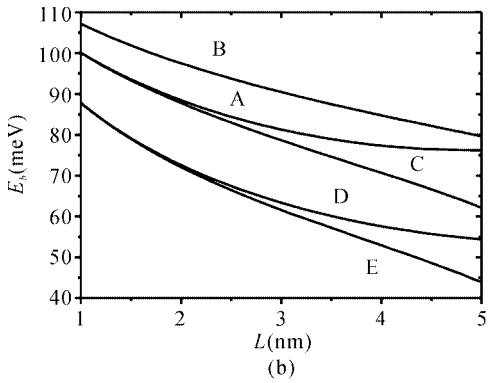


Fig.2 The ground-state donor binding energy E_b as a function of the height L of the GaN/$Al_{0.15}Ga_{0.85}N$ quantum dot with radius R = 5 nm, where the built-in electric field is ignored in (a) and considered in (b). The curves A, B, C, D, and E are for the impurity positions z_i=- L/2, -L/4, 0, L/4 and L/2 nm, respectively

In Fig.3, the donor binding energy E_b is investigated as a function of Al content with the GaN/$Al_xGa_{1-x}N$ quantum dot height L = 4 nm, radius R = 5 nm and z_i = 0 . It is indicated that the binding energy E_b is decreased monotonically with increase of the Al content. The reason is that the increase of the Al content induces the increase of the built-in electric field, and the distance between the electron and the impurity is increased, so the Coulomb interaction is reduced and the donor binding energy of hydrogenic impurity decreases. We also calculated the variation of the binding energy with the quantum dot height L for the Al content x =0.15, 0.20 and 0.

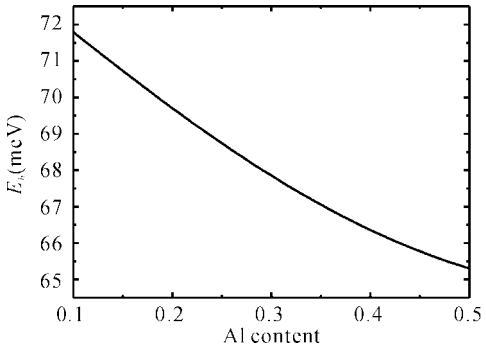


Fig.3 The ground-state donor binding energy E_b as a function of Al content with the GaN/$Al_xGa_{1-x}N$ quantum dot height L = 4 nm, radius R = 5 nm and z_i = 0.

25 (see curves in Fig.4). For small dot height, the change of the binding energy is very small with the Al content x =0.15, 0.20 and 0.25 when the quantum dot height L < 2 nm. The explanation for such a behavior as follows: the spatial quantum confinement becomes strong for small dot height, so the donor binding energy of hydrogenic impurity remains insensitive to the Al content.

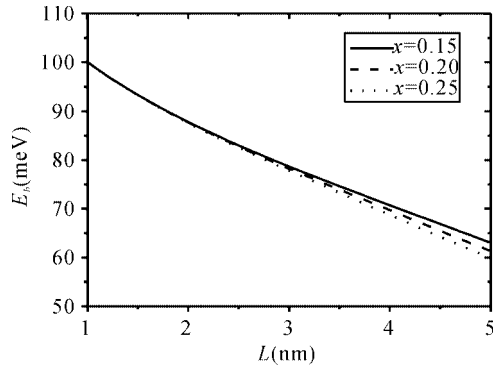


Fig.4 The ground-state donor binding energy E_b as a function of the the GaN/$Al_{0.15}Ga_{0.85}N$ quantum dot height with x = 0.15, 0.20 and 0.25, respectively, and the radius R = 5 nm and z_i = 0

Within the effective-mass approximation and using a variational produce, we have calculated the influence of strain on the ground-state binding energy of a hydrogenic impurity in the WZ GaN/$Al_xGaN_{1-x}N$ strained quantum dot subjected to the built-in electric field for the infinite confinement potential. Numerical results show that the increase of the Al content induces the increase of the built-in electric field, the distance between the electron and the impurity is increased, so the Coulomb interaction is reduced and the donor binding energy of hydrogenic impurity decreases. In particular, for small dot height, the change of the binding energy is very small with the Al content x =0.15, 0.20 and 0.25 when the quantum dot height L < 2 nm. The physical reason is the spatial quantum confinement. Experimental results for hydrogenic donor impurity in WZ GaN/$Al_xGaN_{1-x}N$ strained quantum dot are lacking at present. We hope that our calculation results can stimulate further investigations of the physics, as well as device application of group-III nitrides.

References

[1] S. Nakamura ,G. Fasol, The Blue Laser Diode, Springer-Verlag, Berlin, 1997.

[2] A. Bell ,I. Harrison ,T. S. Cheng ,D. Korakakis, C. T. Foxon, S. Novikov, B. Y. Ber, Y. A. Kudriavtsev, Semicond. Sci. Technol., **15** (2000), 789.

[3] S. Nakamura, M. Senoh, S. Nagahama, T. Matsushita, H. Kiyoku, Y. Sugimoto, T. Kozaki, H. Umemoto, M. Sano, T. Mukai, Jpn. J. Appl. Phys., **38** (1999), L226, Part 2.

[4] G. Bastard. Phys. Rev., B **24** (1981), 4714.

[5] J. L. Zhu, X. Chen, Phys. Rev. B., **50** (1994), 4497.

[6] D. S. Chuu ,C. M. Hsiao ,W. N. Mei, Phys. Rev. B., **46** (1993) ,3898.

[7] N. P. Montenegro, S. T. P. Merchancano, Phys. Rev. B., **46** (1992), 9780.

[8] C. Bose, J. Appl. Phys., **83** (1998), 3089.

[9] C. I. Mendoza, G. J. Vzquez, M. D. C. Mussot, H. N. Spector, Phys. Status Solidi C., **1** (2004), S74.

[10] F. J. Ribeiro, A. Latge, M. Pacheco, Z. Barticevic, J. Appl. Phys., **82** (1997), 270.

[11] J. M. Shi, F. M. Peeters, Phys. Rev. B., 50(1994), 15182.

[12] C. I. Mendoza, G. J. Vazquez, M. D. C. Mussot, H. Spector, Phys. Rev. B., **71** (2005), 075330.

[13] J. L. Movilla, G. J. Planelles, Phys. Rev. B., **71** (2005), 075319.

[14] C. A. Duque, A. L. Morales, A. Montes, Phys. Rev. B., **55** (1996), 10721.

[15] M. Barati, M. R. K. Vahdani, G. Rezaei, J. Phys.: Condens. Matter., **19** (2007), 136208.

[16] Dai Xian Qi, Huang Feng Zhen, Zheng Dong Mei, Chinese Journal of Semiconductors., **26** (2005), 697.