Effects of hydrostatic pressure and external electric field on the impurity binding energy in strained GaN/$Al_xGa_{1-x}N$ spherical quantum dots*

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The binding energy and Stark effect energy shifts of a shallow donor impurity state in a strained GaN/$Al_xGa_{1-x}N$ spherical finite-potential quantum dot (QD) are calculated using a variational method based on the effective mass approximation. The binding energy is computed as a function of dot size and hydrostatic pressure. The numerical results show that the binding energy of the impurity state increases, attains a maximum value, and then decreases as the QD radius increases for any electric field. Moreover, the binding energy increases with the pressure for any size of dot. The Stark shift of the impurity energy for large dot size is much larger than that for the small dot size, and it is enhanced by the increase of electric field. We compare the binding energy of impurity state with and without strain effects, and the results show that the strain effects enhance the impurity binding energy considerably, especially for the small QD size. We also take the dielectric mismatch into account in our work.

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$Al_xGa_{1-x}N$ materials have adjustable band gap ranging from 3.3 eV to 5.1 eV, and the huge mismatch of conduction band in the interface of GaN/$Al_xGa_{1-x}N$ heterojunction is an order of magnitude bigger than the traditional GaAs/$Al_xGa_{1-x}As$ system[1,2]. Therefore, GaN/$Al_xGa_{1-x}N$ is very suitable for the optoelectronic devices operating in the short wavelengths of visible and ultraviolet spectral regions. An external electric field along the growth direction of quantum dots (QDs) can be used to control and modulate the output intensity of the optoelectronic devices, so the function of the electric effect has been widely studied for quantum well[3-5] and DQ[6-9].

Hydrostatic pressure can shift effectively the energy levels of semiconductor materials without altering the crystal symmetry. Because the applied pressure can also modulate the strain effects, it has attracted considerable attention both theoretically and experimentally[10-16].

The topics like confined donors or acceptors in QDs have been extensively investigated[7-21]. Although many authors have discussed the impurity states in GaN/$Al_xGa_{1-x}N$ zinc-blende QDs[18,19], the strain and pressure are neglected in previous works. Thus, further research is meaningful to the design and manufacture of optoelectronic devices.

In this paper, we investigate the effects of external electric field and hydrostatic pressure on the binding energy of a shallow donor impurity in a strained GaN/$Al_xGa_{1-x}N$ spherical finite-potential QD using the variational approach with the effective mass approximation. Our results seem to be more reliable than those obtained before[18,19], since the effects of strain due to the mismatch of lattice constants are considered here.

In the effective mass approximation, the Hamiltonian for impurity state in a spherical QD under the influence of electric field is given by

$$H_I = \frac{-\hbar^2\nabla^2}{2m^*} + V_C(r) + V(r) + e\boldsymbol{F}\cdot\boldsymbol{r} \quad . \tag{1}$$

Similarly, the Hamiltonian for an electron in the absence of the donor can be written as

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$$H_0 = \frac{-\hbar^2\nabla^2}{2m^*} + V_C(r) + e\boldsymbol{F}\cdot\boldsymbol{r} \ , \tag{2}$$

where $\boldsymbol{F}$ is the external electric field along the z-axis, e is the absolute value of the electronic charge, and the effective mass is given by

$$m^* = \begin{cases} m_1, & r \le R \\ m_2, & r \ge R \end{cases} \ , \tag{3}$$

where m_1 and m_2 are the effective masses of GaN and $Al_xGa_{1-x}N$, respectively, and R is the radius of QD. The confining potential $V_C(r)$ is given by

$$V_C(r) = \begin{cases} 0, & r \le R \\ V_0, & r \ge R \end{cases} \ , \tag{4}$$

where V_0 depends on the Al concentration in $Al_xGa_{1-x}N$. $V(r)$ is the Coulomb potential energy within the electron and impurity.

The dielectric constant of the dot is ε_1, and that on the barrier is ε_2. Because of the difference of the dielectric constants, an electron is not only the donor ion itself, but also the image charge distribution. In our presentation, as the spherical symmetry of spherical QD, electric displacement is $\boldsymbol{D} = \frac{e}{4\pi r^2}\boldsymbol{e}_r = \varepsilon\boldsymbol{E}$, so $\boldsymbol{E} = \frac{e}{4\pi r^2}\boldsymbol{e}_r$, where $\boldsymbol{e}_r$ is unit vector along the direction of the radius to outside. So the Coulomb potential is

$$\varphi(r) = \int_0^\infty \boldsymbol{E}\,\mathrm{d}\,\boldsymbol{r} = \begin{cases} \dfrac{e}{4\pi\varepsilon_1 r} - \dfrac{e}{4\pi R}\dfrac{\varepsilon_2-\varepsilon_1}{\varepsilon_1\varepsilon_2}, & r \le R \\ \dfrac{e}{4\pi\varepsilon_2 r}, & r \ge R \end{cases} \ , \tag{5}$$

where ε_1 and ε_2 are the dielectric constants inside and outside the dot, respectively. The Coulomb potential energy is[20]

$$V(r) = -e\varphi(r) = \begin{cases} -\dfrac{e^2}{4\pi\varepsilon_1 r} + \dfrac{e^2}{4\pi R}\dfrac{\varepsilon_2-\varepsilon_1}{\varepsilon_1\varepsilon_2}, & r \le R \\ -\dfrac{e^2}{4\pi\varepsilon_2 r}, & r \ge R \end{cases} \ . \tag{6}$$

Using a variational method, the trial wave functions of Eq. (1) for the ground state of the impurity state can be written as[21]

$$\phi(r) = \begin{cases} \sin(\alpha r)\exp(-\lambda_1 r)\exp(-\lambda_2 r\cos\theta)/r, & r \le R \\ \sin(\alpha R)\exp(\beta R)\exp(-\beta r)\exp(-\lambda_1 r)\exp(-\lambda_2 r\cos\theta)/r, & r \ge R \end{cases} \ , \tag{7}$$

where λ_1 and λ_2 are the variational parameters. $\alpha = \sqrt{2m_1 E_0/\hbar^2}$, and $\beta = \sqrt{2m_2(V_0 - E_0)/\hbar^2}$, where E_0 is the energy of the ground state in the absence of the electic field for an electron and can be solved by the transcendental equation[20]

$$\alpha = \left[\left(1 - m_1/m_2\right)/R - \frac{m_1}{m_2}\beta\right]\tan(\alpha R) \ . \tag{8}$$

From Eq.(8), the smallest radius for the existence of a bound state can be obtained as

$$R_{\min} = \sqrt{\frac{\hbar\pi^2}{4m_1V_0} + \frac{\hbar(m_2/m_1 - 1)^2}{m_2V_0}} \ . \tag{9}$$

Finally, the ground state energy of the impurity state and an electron in the absence of impurity under the electric field are can be obtained by minimizing the expectation energy with respect to λ_1 and λ_2, which are as follows

$$\overline{E}_1 = \min_{\lambda_1,\lambda_2} \frac{\langle\phi(r)|H_1|\phi(r)\rangle}{\langle\phi(r)|\phi(r)\rangle}, \tag{10}$$

$$\overline{E}_0 = \min_{\lambda_1=0,\lambda_2} \frac{\langle\phi(r)|H_0|\phi(r)\rangle}{\langle\phi(r)|\phi(r)\rangle} \ . \tag{11}$$

The binding energy of impurity state for the ground state under electric field is given by

$$E_{\text{ion}} = \overline{E}_1 - \overline{E}_0 \ . \tag{12}$$

The Stark effect energy shift of impurity state energy can be written as

$$\Delta E_{\text{Stark}} = \overline{E}_1(F) - \overline{E}_1(F=0) \ . \tag{13}$$

The variations of the parameters, such as dot size, dielectric constant, effective mass and barrier height, which are caused by the strain effects due to the mismatch of lattice constants and the hydrostatic pressure modifications, are considerable. The variations can automatically affect the donor binding energy and Stark effect energy shift. In the present work, we display the above parameters of GaN and AlN depending on the strain and hydrostatic pressure. The corresponding parameter of $Al_xGa_{1-x}N$ can be obtained by linear interpolation method[22].

The lattice constant depending on the pressure is expressed by Murnaghan state equation[23]:

$$a_j(P) = a_j(0)\left[1 - \frac{P}{3B_{0,j}}\right] \ , \tag{14}$$

where $a_j(0)$ is the j material's lattice constant for zero pressure, and $B_{0,j}$ is the j material's bulk modulus of zinc-bilende structure.

The variations of biaxial and uniaxial strain tensor ratio with pressure can be written as[24]

$$\varepsilon_{xx,j}(P) = \varepsilon_{yy,j}(P) = \frac{a_k(P) - a_j(P)}{a_j(P)} \ , \tag{15}$$

$$\varepsilon_{zz,j}(P) = -2\frac{C_{12,j}}{C_{11,j}}\varepsilon_{xx,j}(P) \quad , \tag{16}$$

where j is GaN($Al_xGa_{1-x}N$) material, k is $Al_xGa_{1-x}N$(GaN) material, and $C_{11,j}$ and $C_{12,j}$ are elastic constants for j material.

The variation of band gap with the hydrostatic pressure P is considered as[23]

$$E_{g,j}(P) = E_{g,j}(0) + bP + cP^2 \quad , \tag{17}$$

where b and c are the pressure coefficient of band gap for GaN or $Al_xGa_{1-x}N$, and the band gap of $Al_xGa_{1-x}N$ for zero pressure obtained by linear interpolation method. In the strained zinc-blende QD, the variation of band gap with the pressure and strain can be written as[24]

$$E_{g,j}(P,\varepsilon) = E_{g,j}(P) + \left(\alpha_j^{C} - \alpha_j^{V}\right)\left[2\varepsilon_{xx,j}(P) + \varepsilon_{zz,j}(P)\right] \quad , \tag{18}$$

where α_j^{C} and α_j^{V} are the deformation potentials of conduction and valence band, respectively.

The variation of electronic effective mass with the pressure and strain can be calculated by[25]

$$\frac{m_e}{m_j} = 1 + \frac{C_j}{E_{g,j}(P,\varepsilon)} \, , \tag{19}$$

where C_j is a constant and can be determined by solving Eq. (20) when P= 0. The hydrostatic pressure dependence of frequencies can be written by the Grüneisen parameter[23].

$$\gamma_{j,i} = B_{0,j}\frac{1}{\omega_{j,i}}\frac{\partial\omega_j(P)}{\partial P} \quad (i = \mathrm{LO,TO}) \, . \tag{20}$$

The modification of phonon energy due to pressure can be expressed as[23]

$$\hbar\omega_{i,j}(P) = \hbar\omega_{i,j}\exp\left(\frac{r_{i,j}}{B_{0,j}}P\right), (i = \mathrm{LO,TO}) \quad . \tag{21}$$

The variations of high frequency dielectric constant with the hydrostatic pressure can be written as[26]

$$\varepsilon_{\infty,j}(P) = 1 + \left[\varepsilon_{\infty,j} - 1\right]\exp\left[\frac{5}{3B_{0,j}}\left(f_{\mathrm{ion},j} - 0.9\right)P\right] \, . \tag{22}$$

Using the famous Lyddane-Sachs-Teller (LST) relationship[24], the static-dielectric constant with pressure effect can be derived as

$$\varepsilon_{0,j}(P) = \varepsilon_{\infty,j}(P)\left[\frac{\hbar\omega_{\mathrm{LO}}}{\hbar\omega_{\mathrm{TO}}}\right]^2 \, . \tag{23}$$

The other parameters with pressure for ternary mixed crystal $Al_xGa_{1-x}N$ can be obtained by linear interpolation method:

$$Q_{Al_xGa_{1-x}N} = (1-x)Q_{GaN} - xQ_{AlN} \quad , \tag{24}$$

where Q_{GaN} and Q_{AlN} are the corresponding parameters associated with GaN and AlN, respectively.

In order to understand the pressure, strain and electric field dependences of the donor binding energy, we preform numerical computation for GaN/$Al_xGa_{1-x}N$ spherical QD. Using the band gap difference[27] of $E_{g,AlGaN}$=$E_{g,GaN}$(1-x)+$xE_{g,AlN}$+530(1-x)x (meV) and assuming 60 % contribution to the conduction band, the value of V_0 is V_0=0.6 ($E_{g,AlGaN}$-$E_{g,GaN}$). The parameters used in the computations are got from Refs. [23,28-30]. The calculated results are presented in Figs.1-5.

Donor binding energy as a function of dot radius is shown in Fig.1, for the cases with and without strain while pressure is P=0. The donor binding energy increases, attains a maximum value, and then decreases as the dot radius increases. It can be understood by the fact that when the dot radius is extremely large, the confining potential has very small influence on the impurity state, and therefore it tends to the free electron case and the binding energy trends to a constant value. As the dot radius becomes very small, one has a δ-function potential with a finite strength, and tunneling effects are enhanced. Hence, the binding energy attains a maximum value. The result is in good agreement with GaAs/AlGaAs QD in Ref.[31]. On the other hand, we observe that the strain effects are more appreciable for narrow dots. It can be explained by the fact that the QD tends to bulk material with the increase of dot size, and therefore the effect of strain due to the mismatch of lattice constants becomes more and more unconspicuous.

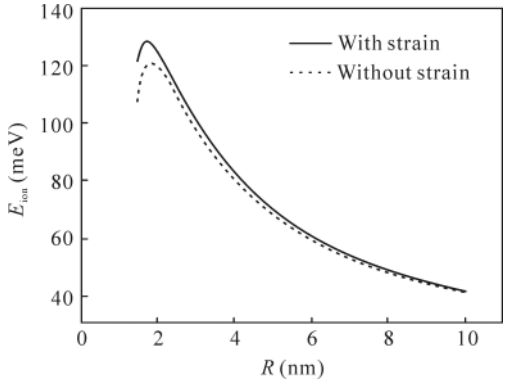

Fig.1 Donor binding energy with and without strain effects as a function of the dot radius

The donor binding energy as a function of Al concentration is shown in Fig.2. It is found that the donor binding energy increases as the Al concentration increasing, and the variation trend is more obvious for the small Al concentration. It can be understood by the fact that the situation tends to the infinite-potential case with the increase of Al concentration, and therefore the effect of barrier height becomes less obvi-

ous for the large Al concentration. In addition, we also notice that the influence of Al concentration is more appreciable for narrow dots. The results can be explained by that the electron feels the boundary of the spherical QD more easily when dot size decreases.

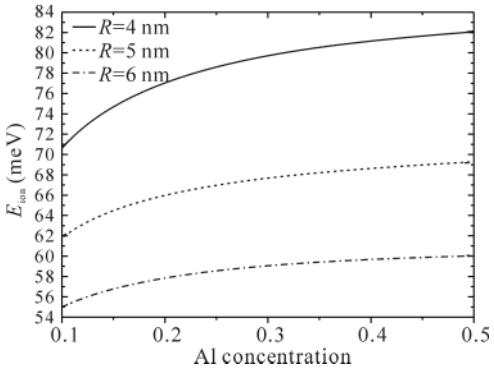

Fig.2 Donor binding energy as a function of Al concentration with different dot radii

Fig.3 shows binding energy of impurity states as a function of the dot radius for different values of the electric field. It is clearly seen that the binding energy hardly changes with respect to the applied electric field in the regime of strong geometric confinement. The binding energy diminishes when the quantum dot confinement decreases, and the behavior becomes stronger as the applied electric field increases. The result is in good agreement with Ref.[18].

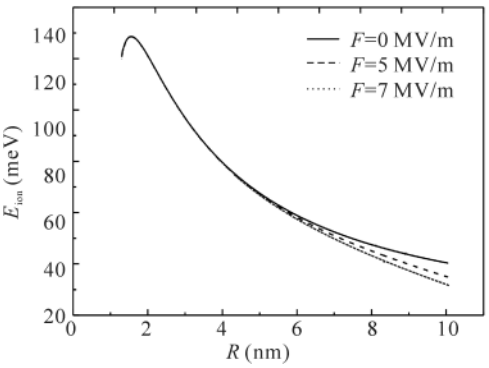

Fig.3 Donor binding energy as a function of the dot radius for three different applied electric fields

In Fig.4, the binding energy is plotted as a function of the hydrostatic pressure for different QD radii. It shows that the impurity binding energy increases nearly linearly with the increasing pressure. It is in good agreement with other works[13-16]. It is explained by the fact that the relative distance between the electron and the impurity is decreased, and then the Coulomb interaction is increased, when the dot size is reduced as the pressure increases. On the other hand, we observe that the influence of pressure is more appreciable for the small dot sizes, which corresponds to the result of C. X. Xia[16].

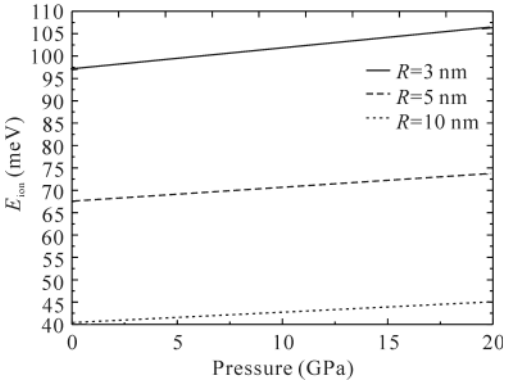

Fig.4 Donor binding energy as a function of the hydrostatic pressure for various dot radii

Fig.5 describes the variation of the energy shift with the field strength. It shows that the Stark shift of impurity energy is increased as the field strength increases. Moreover, we also find that the energy shift increases with increasing dot size. It can be explained by that the influence of electric field is not obvious for the small dot size due to the quantum confinement effect, and therefore the Stark shift is more obvious for the large dot size. The results agree with the result for quantum well[3] and QD[18].

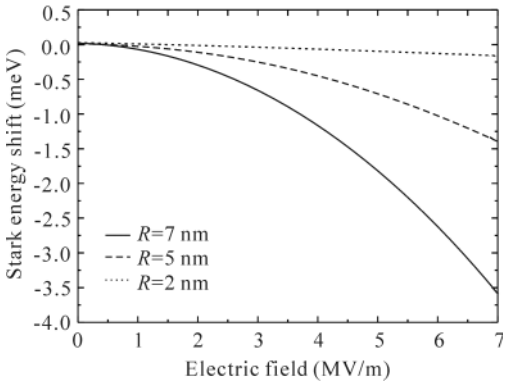

Fig.5 Stark shift of the impurity energy as a function of electric field for various dot radii

To summarize, the binding energy of impurity in a strained zinc-blende GaN/$Al_xGa_{1-x}N$ spherical QD is discussed with a variatioal method by considering the hydrostatic pressure and electric field. The results show that the binding energy of impurities increases with pressure for any dot radius and decreases with the electric filed. The influence of strain effects on the binding energy for small dot radius is stronger than that for large dot radius. The Stark shift of the binding energy of impurity state increases with the electric field, and rapidly becomes larger with increasing dot size.

References

[1] A. D. Bykhovski, B. L. Gelmont and M. S. Shur, J. Appl. Phys. **81**, 6332 (1997).

[2] E. T. Yu, G. J. Sullivan, P. M. Asbeck, C. D. Wang, D. Qiao and S. S. Lau, Appl. Phys. Lett. **71**, 2794 (1997).

[3] Y. C. Li and S. W. Gu, Phys. Rev. B **45**, 12102 (1992).

[4] Y. C. Li and S. W. Gu, J Phys.: Condens. Matter **4**, 135 (1992).

[5] NASHUN Wuritu and GONG Jian, Journal of Optoelectronics • Laser **21**, 1102 (2010). (in Chinese)

[6] C. Bose and C. Chakraborty, Solid-State Electronics **41**,1383 (1997).

[7] Carlos I. Mendoza, G. J. Vazquez, M. del Castillo-Mussot and H. Spector, Phys. Rev. B **71**, 075330 (2005).

[8] Carlos. I. Mendoza, G. J. Vazquez, M. del Castillo-Mussot and Harold N. Spector, Phys. Stat. Sol. C **1**, S74 (2004).

[9] C. Dane, H. Akbas, S. Minez and A. Guleroglu, Physica E **41**, 278 (2008).

[10] S. H. Wei and A. Zunger, Phys. Rev. B **60**, 5404 (1999).

[11] J. M. Wagner and F. Bechstedt, Phys. Rev. B **62**, 4526 (2000).

[12] Z. X. Liu, G. H. Li, H. X. Han and Z. P. Wang, Chinese Journal of Semiconductors **15**, 163 (1994). (in Chinese)

[13] A. M. Elabsy, Physica Scripta **48**, 376 (1993).

[14] G. J. Zhao, X. X. Liang and S. L. Ban, Physics Letters A **319**, 191 (2003).

[15] S. T. Perez-Merchancano, H. Paredes-Gutierrez and J. Silva-Valencia, J. Phys: Condens. Matter **19**, 026225 (2007).

[16] C. X. Xia, F. C. Jiang and S. Y. Wei, Superlattices Microst **43**, 285 (2008).

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

[18] Y. F. Huangfu and Z. W. YAN, Journal of Inner Mongolia University **39**, 18 (2008).

[19] H. T. Wu, H. L. Wang and L. M. Jiang, Acta Physica Sinica **58**, 465 (2009). (in Chinese)

[20] Z. Y. Deng, J. K. Guo and T. R. Lai, J. Phys. Condens. Matter **6**, 5949 (1994).

[21] E. Sadeghi, Physica E **41**, 1319 (2009).

[22] S. Adachi, J. Appl. Phys. **58**, R1 (1985).

[23] Z. W. Yan, S. L. Ban and X. X. Liang, Eur. Phys. J. B **35**, 41 (2003).

[24] L. Shi and Z. W. Yan, Phys. Stat. Sol. C **8**, 42 (2011).

[25] D. Z. Y. Ting and Y. C. Chang, Phys. Rev. B **36**, 4359 (1987).

[26] J. M. Wagner and F. Bechstedt, Phys. Rev. B **66**, 115202 (2002).

[27] H. Wang, G. A. Farias and V. N. Freire, Phys. Rev. B **60**, 5705 (1999).

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

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

[30] N. E. Christensen and I. Gorczyca, Phys. Rev. B **50**, 4397 (1994).

[31] C. Bose and C. Sarkar, Phys. Stat. Sol. B **218**, 461 (2000).