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Calculations of two dimensional electron gas distributions in AlGaN/GaN material system*

Guo Bao-Zeng(郭宝增)[a)†], Gong Na(宫 娜)[a)], and Yu Fu-Qiang(于富强)[b)]

[a)] *College of Electronic and Informational Engineering, Hebei University, Baoding* 071002, *China*
[b)] *College of Physics, Hebei Normal University, Shijiazhuang* 050016, *China*

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This paper presents calculating results of the two-dimensional electron gas (2DEG) distributions in AlGaN/GaN material system by solving the Schrödinger and Poisson equations self-consistently. Due to high 2DEG density in the AlGaN/GaN heterojunction interface, the exchange correlation potential should be considered among the potential energy item of Schrödinger equation. Analysis of the exchange correlation potential is given. The dependencies of the conduction band edge, 2DEG density on the Al mole fraction are presented. The polarization fields have strong influence on 2DEG density in the AlGaN/GaN heterojunction, so the dependency of the conduction band edge on the polarization is also given.

Keywords: GaN, heterojunction, exchange–correlation potential, two-dimensional electron gas
PACC: 7127, 7320D, 7125T

1. Introduction

A unique feature of the AlGaN/GaN material system is the high sheet carrier concentration on the side of GaN in the AlGaN/GaN interface due to large band discontinuities and the spontaneous and piezoelectric polarization.[1−3] Due to the effect of the spontaneous and piezoelectric polarization at interface, high sheet carrier concentration can be obtained even without intentionally doping the barrier. In the AlGaN/GaN MOSFET, this feature of the AlGaN/GaN heterostructures greatly increases the electron concentration in the conduction channel, so the AlGaN/GaN MOSFET can be fabricated for the applications of high current and high power. For this reason, many authors have extensively studied the properties of the two-dimensional electron gas (2DEG) distributions in AlGaN/GaN material system. In order to explore effects of the spontaneous and piezoelectric polarization for the sheet carrier concentration at the AlGaN/GaN interface, Schrödinger's equation can be used self-consistently to couple with Poisson equation. Several approaches can be used to define the system Hamiltonian in the Schrödinger equation, namely envelope function and tight-binding expansion. However, these sophisticated models are only necessary for complex wurtzite band structure, particularly for determining the valence band states. For the simple case of a conduction band with a Γ minimum in nitride-based semiconductors in the wurtzite structure, the simple effective mass approximation (EMA) can be used.

Within the effective mass theory, Schrödinger equation can be defined as

$$\frac{\hbar^2}{2}\frac{\mathrm{d}}{\mathrm{d}z}\left(\frac{1}{m(z)}\frac{\mathrm{d}}{\mathrm{d}z}\right)\psi_i + (qV(z) + \Delta E(z))\psi_i = E_i\psi_i, \quad (1)$$

where $m(z)$ is position dependent effective mass, $V(z)$ is electrostatic potential, $\Delta E(z)$ is band discontinuity, ψ_i is electron wavefunction, E_i is electron energy, $\hbar$ is Planck's constant. Some authors used Eq.(1) and the Poisson equation to study the properties of 2DEG in the AlGaN/GaN interfaces.[4−7]

In some cases the 2DEG density in AlGaN/GaN material system is so high, that the exchange correlation should be considered. In this work, we analysed the expressions of the exchange correlation potential. The exchange correlation potentials were included in the potential energy item of Schrödinger equation. By solving the Schrödinger and Poisson equations self-consistently, the properties of 2DEG in AlGaN/GaN heterojunctions were studied.

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†Corresponding author. E-mail: guobaozeng@yahoo.com.cn

2. Exchange correlation potential[8−12]

Hohenberg, Kohn, and Sham showed that the density distribution of an interacting electron gas under an external field can be obtained by a one-body Schrödinger-type equation containing an exchange–correlation potential $v_{\rm xc}$ in addition to the Hartree potential and the external potential. Such an exchange–correlation potential $v_{\rm xc}$ is given by taking a functional derivative of the exchange–correlation part of the ground-state energy $E_{\rm xc}$ with respect to the number density $n(\boldsymbol{r})$ of electrons. That is

$$v_{\rm xc} = \frac{\delta E_{\rm xc}[n(\boldsymbol{r})]}{\delta n(\boldsymbol{r})}. \tag{2}$$

The functional form of $E_{\rm xc}[n(\boldsymbol{r})]$ is not known and is replaced by a product $n(r)\varepsilon_{\rm xc}(n(\boldsymbol{r}))$ in the usual local density approximation (LDA), where $\varepsilon_{\rm xc}(n(\boldsymbol{r}))$ is the exchange–correlation energy per electron of a uniform electron gas with the density $n(\boldsymbol{r})$. In this approximation $v_{\rm xc}(r)$ becomes the exchange–correlation part of the chemical potential $\mu_{\rm xc}(\boldsymbol{r})$ of the uniform electron gas.

$r_{\rm s}$ is a density parameter. $r_{\rm s}$ can be expressed as

$$r_{\rm s} = \left[\frac{3}{4\pi n}\right]^{1/3}. \tag{3}$$

It is convenient to write in terms of a correlation enhancement factor β

$$v_{\rm xc}(r_{\rm s}) = \beta(r_{\rm s})\mu_{\rm x}(r_{\rm s}), \tag{4}$$

where

$$\begin{aligned} v_{\rm xc}(r_{\rm s}) \cong & \mu_{\rm xc}(r_{\rm s}) = -\frac{e^2}{\pi}\left(3\pi^2\rho\right)^{1/3} \\ = & -\frac{2}{(\pi\alpha r_{\rm s})}{\rm Ryd}, \end{aligned} \tag{5}$$

where Ryd is the unit of Rydberg constant, and $\alpha=[4/(9\pi)]^{1/3}=0.52106$. $\beta(r_{\rm s})$ is expressed as

$$\beta(r_{\rm s}) = 1 + B\chi\ln\left(1+\frac{1}{x}\right), \tag{6}$$

where $B=0.7734$, χ is defined as

$$\chi = \frac{r_{\rm s}}{A}, \tag{7}$$

where $A=21$.

3. Calculation details

By solving the Schrödinger and Poisson equations self-consistently, it is possible to calculate the electron wavefunctions, as well as the energy of each sub-band, occupation of the various sub-band.

The states of the electrons at the perpendicular direction with the AlGaN/GaN interface are quantum, so we can solve one dimension Schrödinger equation at this direction. After the exchange–correlation potential $v_{\rm xc}$ is included, the Schrödinger equation becomes

$$\begin{aligned} & \frac{\hbar^2}{2}\frac{\rm d}{{\rm d}z}\left(\frac{1}{m(z)}\frac{\rm d}{{\rm d}z}\right)\psi_i + (qV(z) \\ & + qv_{\rm xc}(z) + \Delta E(z))\psi_i = E_i\psi_i. \end{aligned} \tag{8}$$

By Eq.(8), we obtain the wavefunctions ψ_i and electron energy E_i. The electron density $n(z)$ can be calculated from ψ_i and E_i.

$$n(z) = \sum_i N_i(z)\left|\psi_i\right|^2, \tag{9}$$

where

$$\begin{aligned} N_i(z) &= \left(\frac{m(z)k_{\rm B}T}{\pi\hbar^2}\right)F_0\left(\frac{E_{\rm F}-E_i(z)}{k_{\rm B}T}\right) \\ &= \left(\frac{m(z)k_{\rm B}T}{\pi\hbar^2}\right)\ln\left[1+{\rm e}^{(E_{\rm F}-E_i)/k_{\rm B}T}\right], \end{aligned} \tag{10}$$

where $k_{\rm B}$ is Boltzmann constant, $E_{\rm F}$ is the Fermi level, and F_0 is the complete Fermi–Dirac integral of order 0.

The electrostatic potential $V(z)$ is determined by a nonlinear Poisson equation

$$\frac{\rm d}{{\rm d}z}\varepsilon\left(\frac{\rm d}{{\rm d}z}V(z)\right) = -e\left[-n+p(V)+N_{\rm D}^+-N_{\rm A}^-\right], \tag{11}$$

where ε is the dielectric constant, p is the hole density, and $N_{\rm D}^+$ and $N_{\rm A}^-$ is the ionized donor and acceptor concentrations.

Due to the effect of the spontaneous and piezoelectric polarization at the AlGaN/GaN interface the high sheet carrier concentration for 2DEG can be obtained. The total polarization charge can be written as $P_{\rm tot}=P_{\rm piezo}+P_{\rm spont}$, where $P_{\rm piezo}$ is the piezoelectric charge caused by the lattice mismatch and by the thermal strain ($P_{\rm piezo}=P_{\rm mis}+P_{\rm ts}$), whereas $P_{\rm spont}$ represents the spontaneous polarizability of the AlGaN/GaN interface.

The direction of the spontaneous polarization $P_{\rm spont}$ is opposite with the growth [0001] direction of AlGaN/GaN heterojunction, and the value of $P_{\rm spont}$ is negative.

The piezoelectric polarization $P_{\rm piezo}$ can be expressed as

$$P_{\rm piezo} = 2\frac{a-a_0}{a_0}\left(e_{31} - e_{33}\frac{C_{13}}{C_{33}}\right), \qquad (12)$$

where a_0 and a are the lattice constant of the substrate and the epilayer material. e_{31} and e_{33} are the piezoelectric constants. C_{12} and C_{33} are the elastic modules.

The total electric polarization P in $Al_xGa_{1-x}N$ and GaN are given by

$$P_{\rm AlGaN} = P_{\rm spont}({\rm AlGaN}) + P_{\rm piezo}({\rm AlGaN}) \qquad (13)$$

and

$$P_{\rm GaN} = P_{\rm spont}({\rm GaN}) + P_{\rm piezo}({\rm GaN}). \qquad (14)$$

For the AlGaN/GaN heterojunction with the growth of AlGaN on GaN, due to no strain in the GaN, $P_{\rm piezo}$ (GaN) is equal to zero. Because the in-plane constant of AlGaN is always smaller than that of the GaN, the value of $P_{\rm piezo}$ (AlGaN) is negative.

The difference in the electric polarizations is then

$$\begin{aligned}\Delta P &= P_{Al_xGa_{1-x}N} - P_{\rm GaN} \\ &= P_{\rm pizeo}(Al_xGa_{1-x}N) \\ &\quad + P_{\rm spont}(Al_xGa_{1-x}N) - P_{\rm spont}({\rm GaN}) \\ &= 2\frac{a_0 - a(x)}{a(x)}\left(e_{31}(x) - e_{33}(x)\frac{C_{13}(x)}{C_{33}(x)}\right) \\ &\quad + P_{\rm spont}(Al_xGa_{1-x}N) - P_{\rm spont}({\rm GaN}). \qquad (15)\end{aligned}$$

For the case of Ga-face polarization, the density of the fixed positive polarization charges in the AlGaN/GaN interface is $|\Delta P/e|$, where e is the electron charge. The fixed positive polarization charges result in the high sheet density 2DEG on the side of GaN in the AlGaN/GaN interface.

Table 1 shows the material parameters of the AlN and GaN to be used in the calculations of 2DEG.

Table 1. The material parameters of the AlN and GaN.

property	AlN	GaN
bandgap/eV	6.2	3.4
lattice constant a_0/nm	0.3112	0.3189
static dielectric constants ε_0	8.5	8.9
piezoelectric polarization $P_{\rm spont}/({\rm C/m^2})$	−0.081	−0.029
piezoelectric constant $e_{31}/({\rm C/m^2})$	−0.58	−0.36
piezoelectric constant $e_{33}/({\rm C/m^2})$	1.55	1
elastic module c_{31}/Gpa	158	99
elastic module c_{33}/Gpa	267	389
electron effective mass ratio/$(m_{\rm e}^*/{\rm m_0})$	0.48	0.2
hole effective mass ratio/$(m_{\rm h}^*/{\rm m_0})$	4.41	1.96

The calculated bandgaps as a function of Al composition were obtained from the relation

$$E_{\rm g}(x) = E_{\rm g}({\rm GaN})(1-x) + E_{\rm g}({\rm AlN})x - bx(1-x), \qquad (16)$$

where x is the AlN mole fraction and b is the bowing parameter with value 0.96 eV.

The other material parameters of $Al_xGa_{1-x}N$ have been obtained by linear interpolation of the binary compound value x

$$P(Al_xGa_{1-x}N) = P({\rm GaN}) + x(P({\rm AlN}) - P({\rm GaN})), \qquad (17)$$

where P represents the any material parameters of the binary or ternary alloy compound for GaN and AlGaN.

The conduction band offset $\Delta E_{\rm c}$ is determined by

$$\Delta E_{\rm c} = 0.7[E_{\rm g}(Al_xGa_{1-x}N) - E_{\rm g}({\rm GaN})]. \qquad (18)$$

4. Calculated results and discussions

Figure 1 shows the calculated $Al_xGa_{1-x}N$/GaN structure in this work. The $Al_xGa_{1-x}N$/GaN heterojunction is grown in the [0001] direction. The polarization induced fixed charges is in GaN-face. The structure consists of (moving from the gate contact to the substrate) a 45nm n-doped $Al_xGa_{1-x}N$, where x is varied between 0.1 to 0.4, 5nm unintentionally dope AlGaN, and 150nm unintentionally doped GaN layers. We consider a residual doping of $10^{17}{\rm cm^{-3}}$ both GaN

and AlGaN layers. Schottky barrier height of 1.2eV for metal–AlGaN interface is assumed.

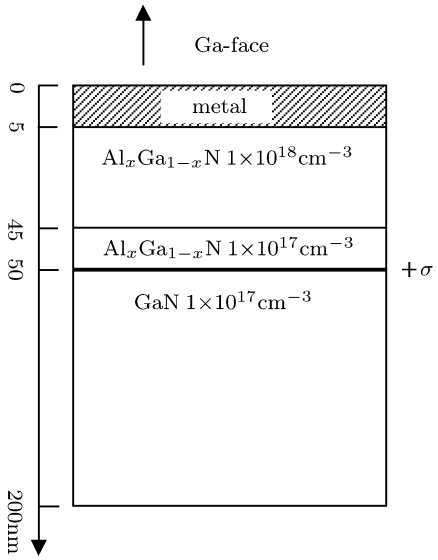


Fig.1. Calculated $Al_xGa_{1-x}N$/GaN structure.

In order to analyse the effect of the exchange–correlation potential on the total Schrödinger potential, Fig.2 shows the one dimension distributions of the exchange–correlation potentials at several different Al composition x in the $Al_xGa_{1-x}N$/GaN structure. It is seen that the exchange–correlation potential increases with the increasing Al composition x, and reaches its maximum value on the side of GaN in the $Al_xGa_{1-x}N$/GaN interface. This is because the band offset ΔE_c increases with the increasing Al composition x, and the increase of the ΔE_c causes the increase of 2DEG density. According to Eqs.(4) and (5), we know that the exchange–correlation potential is proportional to 2DEG density $\rho^{1/3}$, so the maximum 2DEG density and the maximum exchange–correlation potential occur at the same position in the $Al_xGa_{1-x}N$/GaN structure.

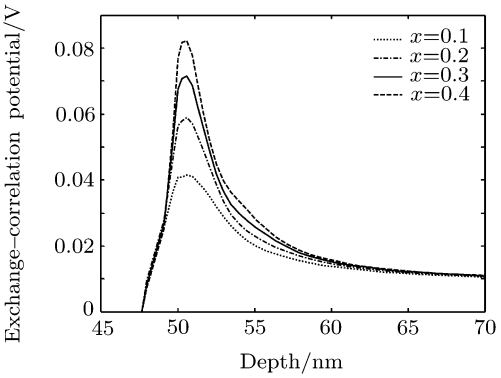


Fig.2. The exchange–correlation potential distribution.

For comparison, the conduction band edges of the $Al_xGa_{1-x}N$/GaN heterojunction considering and without considering the exchange–correlation potential are shown in Fig.3. Here we considered the case of the flat band (no contact potential). Al mole fraction x in the $Al_xGa_{1-x}N$/GaN heterojunction was chosen as 0.3. It is seen that the conduction band edges are lower for considering the exchange–correlation potential than without considering the exchange–correlation potential near the interface of $Al_xGa_{1-x}N$/GaN.

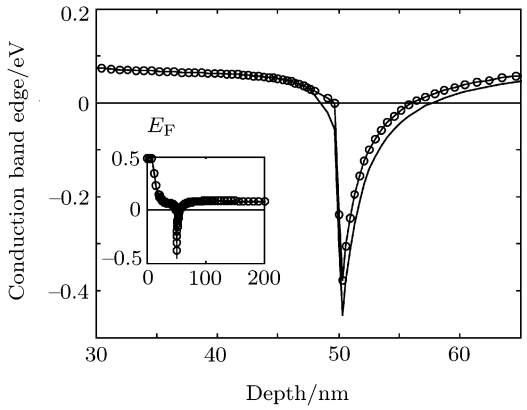


Fig.3. The conduction band edge of the $Al_{0.3}Ga_{0.7}N$/GaN heterojunction. Solid line: considering the exchange–correlation potential; Circle marker line: no considering the exchange–correlation potential. Inset is the same figure as the main figure, but with longer-range coordinate.

As discussed above, the exchange–correlation potential affects the conduction band edge of the $Al_xGa_{1-x}N$/GaN material system, so in our calculations the exchange–correlation potential is considered in the total Schrödinger potential.

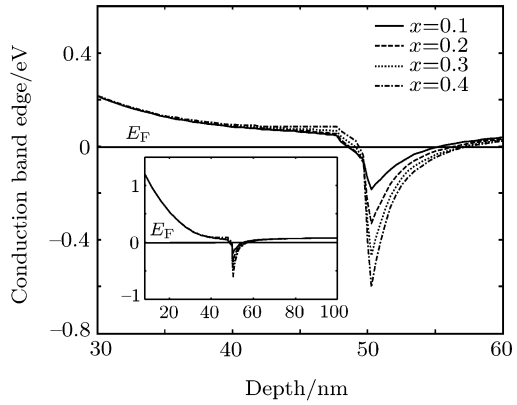


Fig.4. The conduction band edge of the $Al_xGa_{1-x}N$/GaN heterojunction considering the exchange–correlation potential as a function of Al mole fraction. Inset is the same figure as the main figure, but with longer-range coordinate.

Figure 4 shows the conduction band edge profile of the $Al_xGa_{1-x}N/GaN$ heterojunction at various Al mole fraction x. Here Schottky barrier height of 1.2 eV for metal–AlGaN interface is assumed. The depth of the electron barrier well increases with the increase of Al mole fraction x of the AlGaN. It is because the conduction band offset ΔE_c increases with the increase of Al mole fraction x, which is given by Eq.(8).

Polarization effects are quite important for the conduction band edge profile and 2DEG density in the $Al_xGa_{1-x}N/GaN$ heterojunction. We calculated the conduction band edge profile at several different cases of the polarization shown in Fig.5. Due to the polarization, the conduction band edge near the $Al_xGa_{1-x}N/GaN$ heterojunction becomes lower. It is seen that for the case without considering any polarization the most part of the conduction band edge profile is higher than Fermi level E_F, and for the case with considering both the spontaneous and piezoelectric polarization the lowest conduction band edge is –0.27 eV below Fermi level E_F. For the cases with only the spontaneous and only piezoelectric polarization the conduction band edge profile are also given in Fig.5.

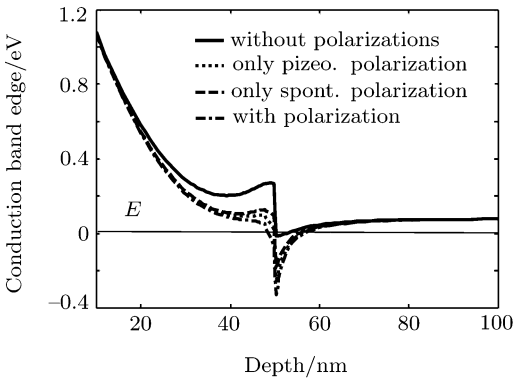


Fig.5. Conduction band edge of the $Al_{0.2}Ga_{0.8}N/GaN$ heterojunction with and without polarization fields.

The polarization field dramatically increases the 2DEG density in the $Al_xGa_{1-x}N/GaN$ heterojunction. As above-mentioned, for the case without considering polarization fields, the most part of the conduction band edge profile is higher than Fermi level E_F. It indicates that the 2DEG density is low. For our calculations of the 2DEG density, the polarization field including spontaneous and piezoelectric polarization is included. The distributions of the 2DEG density at various Al mole fraction x are shown in Fig.6. It is seen that the 2DEG density reaches its maximum value at the interface of heterojunction. The 2DEG density strongly depends on the Al mole fraction x. The maximum values of the 2DEG density at Al mole fraction x=0.1, 0.2, 0.3 and 0.4 are equal to $1.5\times10^{19}cm^{-3}$, $4.2\times10^{19}cm^{-3}$, $7.7\times10^{19}cm^{-3}$ and $1.2\times10^{20}cm^{-3}$, respectively.

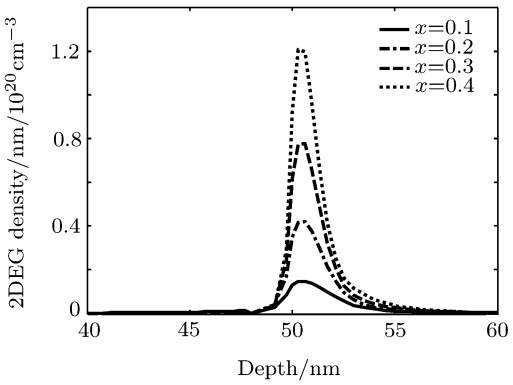


Fig.6. The distribution of 2DEG density as a function of Al mole fraction.

Figure 7 shows the distribution of 2DEG density as a function of Al mole fraction obtained by Sacconi *et al* in Ref.[7]. We can make the comparison between our results in Fig.6 and Sacconi's results in Fig.7. For the calculations of Sacconi *et al* the structure sizes of the device are different from our device, so the horizontal coordinate in Fig.7 is different from the horizontal coordinate in Fig.6. In addition the device parameters in Fig.6 and in Fig.7 may have a little difference. For the Sacconi's results the exchange–correlation potential was not considered. It is seen that the distributions of 2DEG density are approximately the same. It seems to indicate that the exchange–correlation potential do not obviously affect the distribution of 2DEG density. But we think that the effect of the exchange–correlation potential to the density 2DEG exists. Due to the differences of the parameters to be chosen in our calculations and Sacconi's calculations, the densities of 2DEG for our calculations are not larger than for Sacconi's calculations.

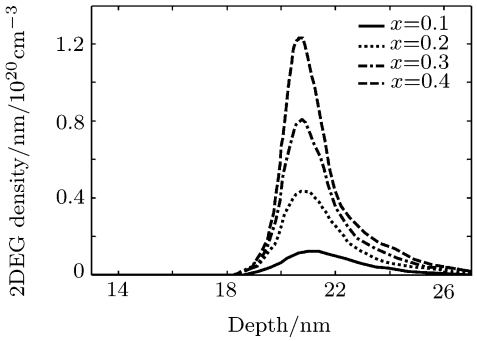


Fig.7. The distribution of 2DEG Density as a function of Al mole fraction in Ref.[7].

The 2DEG sheet density as a function of Al mole fraction in the $Al_xGa_{1-x}N/GaN$ heterojunction is shown in Fig.8. The 2DEG sheet density increases with increasing Al mole fraction which is roughly linear. The 2DEG sheet density at the several Al mole fraction is listed in Table 2.

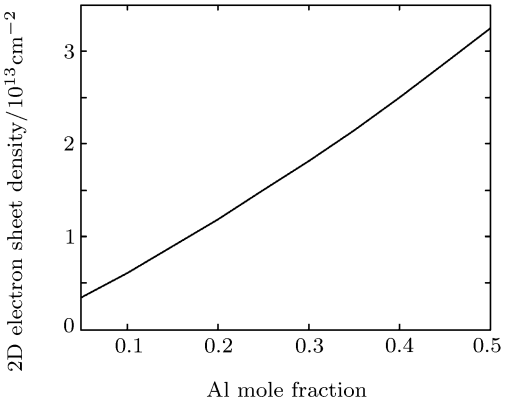


Fig.8. 2DEG sheet density as a function of Al mole fraction.

Table 2. 2DEG sheet density at the several Al mole fraction.

Al mole fraction x	2DEG sheet density/cm^{-2}
0.1	6.07×10^{12}
0.2	1.17×10^{13}
0.3	1.82×10^{13}
0.4	2.50×10^{13}
0.5	3.24×10^{13}

5. Conclusions

By solving the Schrödinger and Poisson equations self-consistently, we calculated the electron wavefunctions, as well as the conduction band edge, 2DEG density in the $Al_xGa_{1-x}N/GaN$ heterojunction. For the potential item in Schrödinger equation the exchange–correlation potential is included. The dependencies of the conduction band edge, 2DEG density on the Al mole fraction are shown. The dependency of the conduction band edge on the polarization field is also given. It indicates that the conduction band edge and 2DEG density strongly depend on the polarization field.

References

[1] Sheppard S T, Doverspike K, Pribble W L, Allen S T, Palmour J W, Kehias L T and Jenkins T J 1999 *IEEE Electron Device Lett.* **20** 161

[2] Yu Tsung-Hsing and Brennan K F 2003 *IEEE Trans. Electron Devices* **50** 315

[3] Chang Y C, Zhang Y M and Zhang Y M 2006 *Chin. Phys.* **15** 636

[4] Kong Y C, Zheng Y D, Zhou C H, Deng Y Z, Gu S L, Shen Bo, Zhang R, Han P, Jiang R L and Shi Y 2004 *Acta Phys. Sin.* **53** 2320 (in Chinese)

[5] Zhang J F, Wang C, Zhang J C and Hao Y 2006 *Chin. Phys.* **15** 1061

[6] Kong Y C, Zheng Y D, Chu R M and Gu S L 2003 *Acta Phys. Sin.* **52** 1756 (in Chinese)

[7] Sacconi F, Carlo A D, Lugli P and Morkoc H 2001 *IEEE Trans. Electron Devices* **48** 450

[8] Hedin L and Lundqvist I 1971 *J. Phys.* C *Solid State Phys.* **4** 2064

[9] Trellakis A and Ravaioli U 1998 *Electrochemical Society Proceedings* **98–19** 551

[10] Trellakis A and Ravaioli U 2002 *J. Appl. Phys.* **92** 3711

[11] Ando T 1976 *Phys. Rev.* B **13** 3468

[12] Trellakis A and Ravaioli U 2004 *Solid-State Electronics* **48** 367