Temperature effects on interface polarons in a strained (111)-oriented zinc-blende GaN/AlGaN heterojunction under pressure*

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Abstract: The properties of interface polarons in a strained (111)-oriented zinc-blende GaN/$Al_xGa_{1-x}N$ heterojunction at finite temperature under hydrostatic pressure are investigated by adopting a modified LLP variational method and a simplified coherent potential approximation. Considering the effect of hydrostatic pressure on the bulk longitudinal optical phonon mode, two branches interface-optical phonon modes and strain, respectively, we calculated the polaronic self-trapping energy and effective mass as functions of temperature, pressure and areal electron density. The numerical result shows that both of them near linearly increase with pressure but the self-trapping energies are nonlinear monotone increasing with increasing of the areal electron density. They are near constants below a range of temperature whereas decrease dramatically with increasing temperature beyond the range. The contributions from the bulk longitudinal optical phonon mode and one branch of interface optical phonon mode with higher frequency are important whereas the contribution from another branch of interface optical phonon mode with lower frequency is extremely small so that it can be neglected in the further discussion.

Key words: polaron; strained zinc-blende heterojunction; temperature; pressure
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1. Introduction

Polaronic properties may influence carrier transportation of semiconductors, and consequently affect the properties of optical-electronic devices. In recent years, the physical properties of quantum heterostructures composed of the group-III nitrides semiconductors with wide-band-gaps, such as AlN, GaN, and InN, and their ternary compounds, are widely studied arising from their promising application in short-wavelength electroluminescence devices[1,2]. Up to now, most works on polaronic properties have been devoted at zero-temperature limit. It was found that the polaronic properties of layered semiconductors such as heterojunctions and quantum wells (QWs) are obviously different from those of bulk materials. In an early year of the last decade, Ban *et al.*[3] studied the temperature dependence of N-dimensional polarons to show their dimensional effect, and it was found that the temperature effect of polarons diminishes with increasing dimensionality. Later, Qin and Gu[4] studied the temperature dependence of polaron self-energy for a polar-crystal slab. It is shown that the self-energy is a decreasing function of temperature. Recently, Hua *et al.*[5] studied the self-energies and effective masses of polarons in a heterostructure. In the last few years, much attention has been paid to the strain effect due to the interface lattice mismatch which influences dramatically the property of semiconductor heterostructures. The strained-induced piezoelectric polarization can also produce a large built-in electric field. Wagner *et al.*[6] studied the dielectric, lattice-dynamical, and electronic properties of biaxially and uniaxially strained group-III nitrides. Sánchez-Rojas *et al.*[7] presented the internal electric field distributions in AlGaN/GaN and InGaN/GaN heterostructures. As much as we know, there is still a lack about the temperature effect of polarons in strained zinc-blende nitride heterojunctions.

High pressure technology has also become an important tool in determining the band structures and understanding the electronic and optical properties of bulk semiconductors and heterostructures. The hydrostatic pressure effect on the binding energies of donors and exciton in heterojunctions and QWs were given by Ban and Liang[8,9]. The result showed that the binding energies increase with pressure obviously. Wagner *et al.*[10] calculated the dielectric and lattice-dynamical properties of zinc-blende and wurtzite GaN and AlN under hydrostatic pressure. In experiment, Goñi *et al.*[11] investigated the pressure behavior of phonon modes on the hexagonal (wurtzite) and cubic (zinc-blende) modifications of GaN and hexagonal AlN, respectively. More recently, we discussed the Stark effect of impurity states of donors in strained nitride heterojunctions with the zinc-blende structure to show the pressure effect[12].

This paper is focused on the temperature and hydrostatic pressure effect on the self-trapping energies and effective masses of polarons in a strained zinc-blende nitride heterojunction by considering the influence of half-space bulk longitudinal (LO) and two interface-optical (IO) phonon modes. Meanwhile, the effect of the electronic wave function penetrating into the barrier regions is also taken into account. We ex-

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tend a simplified coherent potential approximation[13] (SCPA) to obtain some physical parameters for a ternary mixed crystal of nitrides in the III-V group. The results show that the effect of temperature make the polaron self-trapping energy decrease obviously so that the polaron becomes free electron-like as temperature increases beyond some value. On the other hand, it is also found that the comprehensive effect of pressure on the physical factors of a heterojunction induces the polaronic self-trapping energy to increase near linearly with pressure. The temperature and pressure influence distinctly on the polaron effective mass with a trend similar to that of self-trapping energy.

2. Model and calculation

In this work, we consider a strained (111)-oriented zinc-blende GaN/$Al_xGa_{1-x}N$ realistic heterojunction with GaN layer as the channel side, denoted by material 1 and located at $z > 0$. The barrier side is $Al_xGa_{1-x}N$ which is assumed to be infinite, denoted by material 2 and located at $z < 0$. The interface of the heterojunction is defined as the $x-y$ plane. By considering the interaction from the LO and IO phonons, the Hamiltonian of this system can by written as[13]

$$H = H_{x-y} + H_z + H_{\text{ph}} + H_{\text{e-ph}}, \tag{1}$$

where

$$H_{x-y} = \frac{p_x^2 + p_y^2}{2m_{//1}}\theta(z) + \frac{p_x^2 + p_y^2}{2m_{//2}}\theta(-z) \tag{2a}$$

$$H_z = \frac{p_z^2}{2m_{\perp 1}}\theta(z) + \frac{p_z^2}{2m_{\perp 2}}\theta(-z) + V(z) \tag{2b}$$

$$\begin{aligned} H_{\text{ph}} = &\sum_{\boldsymbol{k}} \hbar\omega_{\text{L}1} a_{\boldsymbol{k}1}^+ a_{\boldsymbol{k}1}\theta(z) + \sum_{\boldsymbol{k}} \hbar\omega_{\text{L}2} a_{\boldsymbol{k}2}^+ a_{\boldsymbol{k}2}\theta(-z) \\ &+ \sum_{\boldsymbol{q},\sigma} \hbar\omega_\sigma b_{\boldsymbol{q}\sigma}^+ b_{\boldsymbol{q}\sigma}, \end{aligned} \tag{2c}$$

and

$$\begin{aligned} H_{\text{e-ph}} = &\sum_{\boldsymbol{k}} \left[\frac{1}{k} \sum_{\lambda} B_\lambda(z) \sin(k_z |z|) \mathrm{e}^{-i(\boldsymbol{k}_{//}\cdot\boldsymbol{\rho})} a_{\boldsymbol{k}}^+ + h.c. \right] \\ &+ \sum_{\boldsymbol{q},\boldsymbol{\sigma}} \left\{ \left[\frac{G_\sigma}{\sqrt{q}} \left(\mathrm{e}^{-i(\boldsymbol{q}\cdot\boldsymbol{\rho})} \mathrm{e}^{-q|z|} \right) \right] b_{\boldsymbol{q}\sigma}^+ + h.c. \right\}. \end{aligned} \tag{2d}$$

All of the parameters used in the above equations were defined in our previous work[13].

The trial wave function for the electron phonon system can be chosen as follows[3]:

$$\begin{aligned} \left| P, \{n_\sigma(q)\}, \{n_{k,\lambda}(k)\} \right\rangle = &\exp(s_1)\exp(s_2)\exp\left\{ \frac{i}{\hbar} \left[\boldsymbol{p} - \hbar \sum_{k\lambda} n_{k,\lambda}(k)\theta(\lambda, z)\boldsymbol{k}_{//} \right. \right. \\ &\left. \left. -\hbar \sum_{q\sigma} n_\sigma(q)\boldsymbol{q} \right] \cdot \boldsymbol{\rho} \right\} \cdot \sum_{\boldsymbol{q}\sigma} \frac{\left(b_{\boldsymbol{q}\sigma}^+\right)^{n_\sigma(q)}}{\left[n_\sigma(q)!\right]^{1/2}} \prod_k \frac{\left(a_{\boldsymbol{k}\lambda}^+\right)^{n_\lambda(k)}}{\left[n_{k,\lambda}(k)!\right]^{1/2}} |\xi(z)\rangle \left|0_{\boldsymbol{q},\sigma}\right\rangle \left|0_{\boldsymbol{k},\lambda}\right\rangle, \end{aligned} \tag{3}$$

where $|0\rangle$ is the vacuum state of phonons, and $|\xi(z)\rangle$ is the electronic function in the z direction.

$$\xi(z) = \begin{cases} \xi_1(z) = Bb^{1/2}(bz+\beta)\exp(-bz/2), & z > 0, \\ \xi_2(z) = Dd^{1/2}\exp(bz/2), & z < 0, \end{cases} \tag{4}$$

where b, d are the variational parameters, and the normalization constants in the above equation satisfy $\beta = 2b/(b+d)$, $B = [\beta^2(1 + b/d) + 2\beta + 2]^{-1/2}$ and $D = B\beta(b/d)^{1/2}$.

In Eq. (3), the two exponential functions are the operators of displacement oscillators:

$$\exp(s_1) = \exp\left[\frac{i}{\hbar} \left(-\hbar \sum_{\boldsymbol{k}} \boldsymbol{k}_{//} a_{\boldsymbol{k}\lambda}^+ a_{\boldsymbol{k}\lambda}\theta(\lambda, z) - \hbar \sum_{\boldsymbol{q},\sigma} \boldsymbol{q} b_{\boldsymbol{q}\sigma}^+ b_{\boldsymbol{q}\sigma} \right) \cdot \boldsymbol{\rho} \right] \tag{5a}$$

and

$$\begin{aligned} &\exp(s_2) = \\ &\exp\left[\sum_{\boldsymbol{k},\lambda} \left(f_{\boldsymbol{k}\lambda} a_{\boldsymbol{k}\lambda}^+ - f_{k\lambda}^* a_{\boldsymbol{k}\lambda} \right)\theta(\lambda, z) + \sum_{\boldsymbol{q},\sigma} \left(g_{q\sigma} b_{\boldsymbol{q}\sigma}^+ - g_{q\sigma}^* b_{\boldsymbol{q}\sigma} \right) \right]. \end{aligned} \tag{5b}$$

$\{n_{k,\lambda}(k)\} = n_\lambda(k_1), n_\lambda(k_2), \cdots, n_\lambda(k_i)$ are the thermo-phonon numbers corresponding to different wave vectors $\boldsymbol{k}_i$ of the bulk phonon modes. $\{n_\sigma(q)\} = n_\sigma(q_1), n_\sigma(q_2), \cdots, n_\sigma(q_j)$ are the thermo-phonon numbers corresponding to different wave vectors q_i of the interface phonon modes. $\boldsymbol{P}$ is the total momentum of the system and $\rho = \sqrt{x^2 + y^2}$. If we adopt the orthogonal and complete set of the non-interaction eigen-states (3), the partition function of the system can be determined using Peierls' variational principle

$$Z = T_{\text{r}}\exp(-H/k_{\text{B}}T) \geqslant \sum_n \exp(-\langle n|H|n\rangle/k_{\text{B}}T), \tag{6}$$

where $|n\rangle$ denotes the eigenstate of the non-interactions system. The polaronic energy can be written as

$$E = E_1 + E_2, \tag{7}$$

in which

$$E_1 = \langle\xi(z)| + \frac{p_z^2}{2m_{\perp 1}}\theta(z) + \frac{p_z^2}{2m_{\perp 2}}\theta(-z) + V(z)|\xi(z)\rangle, \tag{8a}$$

where the detailed quantity of E_1 were given in Ref. [13].

$$E_2 = \langle P, \{n_\sigma(q)\}, \{n_\lambda(k)\}| H_2 |P, \{n_\sigma(q)\}, \{n_\lambda(k)\}\rangle. \tag{8b}$$

For a polaron with a fixed momentum $\boldsymbol{K}_{\text{p}} = \boldsymbol{P} - \hbar\sum_{k,\lambda} \boldsymbol{k}_{//} n_\lambda(k) - \hbar\sum_{q,\sigma} \boldsymbol{q} n_\sigma(q)$, we can obtain the total par-

tition function:

$$Z_{\rm p} = \sum_{P,\{n_{k,\lambda}(k)\},\{n_\sigma(q)\}} \exp\left[-\frac{1}{k_{\rm B}T}E(\bar{P},\{n_{k,\lambda}(k)\},\{n_\sigma(q)\})\right] \times \delta\left[\boldsymbol{P} - \hbar\sum_k \boldsymbol{k}_{//} n_{\boldsymbol{k},\lambda}(k) - \hbar\sum_{\boldsymbol{q}\sigma}\boldsymbol{q}n_\sigma(q) - \boldsymbol{K}_p\right]. \quad (9)$$

The free energy of the system can be written as

$$E_{\rm p} = -k_{\rm B}T\ln Z_{\rm p}. \quad (10)$$

It was proved that $n_{{\rm k},\lambda}(k)$, and $n_\sigma(q)$ are insensitive to $|f_{k\lambda}|^2$ and $\left|g_{q\sigma}\right|^2$ respectively, so that the thermo-phonon numbers can be replaced by that with wave vectors $\boldsymbol{q} = 0$ and $\boldsymbol{k} = 0$.

$$n_{k,1}(0) = \frac{1}{\exp\left(\dfrac{\hbar\omega_{\rm L1}\overline{P_1}}{k_{\rm B}T}\right) - 1} \quad (11a)$$

$$n_{k,2}(0) = \frac{1}{\exp\left(\dfrac{\hbar\omega_{\rm L2}\overline{P_2}}{k_{\rm B}T}\right) - 1} \quad (11b)$$

and

$$n_\sigma(0) = \frac{1}{\exp\left(\dfrac{\hbar\omega_\sigma}{k_{\rm B}T}\right) - 1}, \quad (11c)$$

where $\overline{P_1} = \int_0^\infty |\xi_1(z)|^2{\rm d}z$, and $\overline{P_2} = \int_{-\infty}^0 |\xi_2(z)|^2{\rm d}z$ are the electron probabilities in materials 1 and 2, respectively.

Then Equation (8b) can be written as

$$E_2 = \frac{1}{2m^*}\boldsymbol{K}_p^2 - \sum_k \frac{|\phi_{\rm A}|^2}{\left\{\hbar\omega_{\rm L1}\overline{P_1} + \dfrac{\hbar^2k_{//}^2\overline{P_1}}{2m_{//1}}\left[2n_{k,1}(0)+1\right] + \hbar\omega_{\rm L2}\overline{P_2} + \dfrac{\hbar^2k_{//}^2\overline{P_2}}{2m_{//2}}\left[2n_{k,2}(0)+1\right]\right\}} - \sum_{q\sigma}\frac{|\phi_{\rm G}|^2}{\left\{\hbar\omega_\sigma + \dfrac{\hbar^2q^2}{2m_{//}}\left[2n_\sigma(0)+1\right]\right\}}, \quad (12)$$

where

$$\phi_{\rm A} = \langle\psi|\frac{A}{k}\sin(k_z z)|\psi\rangle \quad (13a)$$

and

$$\phi_{\rm G} = \langle\psi|\frac{G_\sigma}{\sqrt{q}}{\rm e}^{-qz}|\psi\rangle. \quad (13b)$$

We minimize $E(b,d)$ to obtain the ground state energy $E_{\rm P}$ for a polaron. Choosing $E_2 = 0$ and using the same process, the bound energy or self-trapping energy of a polaron can be written as

$$E_{\rm B} = E_{\rm f} - E_{\rm p}. \quad (14)$$

The polaron effective mass is reduced to be

$$m^* = m(1 + \Delta m_{\rm LO} + \Delta m_{{\rm I}\sigma}), \quad (15)$$

where

$$\Delta m_{\rm LO} = \frac{2\hbar^2}{m_{//}}\sum_k \frac{|\phi_{\rm A}|^2 k_{//}^2\cos^2\theta}{\left\{\hbar\omega_{\rm L1}\overline{P_1} + \dfrac{\hbar^2k_{//}^2\overline{P_1}}{2m_{//1}}\left[2n_{k,1}(0)+1\right] + \hbar\omega_{\rm L2}\overline{P_2} + \dfrac{\hbar^2k_{//}^2\overline{P_2}}{2m_{//2}}\left[2n_{k,2}(0)+1\right]\right\}^3} \quad (16a)$$

and

$$\Delta m_{{\rm I}\sigma} = \frac{2\hbar^2}{m_{//}}\sum_{q,\sigma}\frac{|\phi_{\rm G}|^2 q^2\cos^2\theta}{\left\{\hbar\omega_\sigma + \dfrac{\hbar^2q^2}{2m_{//}}\left[2n_\sigma(0)+1\right]\right\}^3}. \quad (16b)$$

3. Pressure coefficients

Considering the biaxial, uniaxial strain and the modulation of hydrostatic pressure on the electronic effective mass, dielectric constants and the band offset in GaN and $Al_xGa_{1-x}N$, the relevant parameters are expressed as the following forms.

For the GaN material with finite thickness, the biaxial lattice-misfit-induced strains are given as

$$\varepsilon(p) = \varepsilon_{xx} = \varepsilon_{yy} = \frac{a_2(P) - a_1(P)}{a_1(P)}$$
$$\varepsilon_{zz} = -D_{111}\varepsilon_{xx} \quad (17)$$

where D_{111} is the strain module with (111) orientation and given as

$$D_{111}(P) = -\frac{C_{11}(P) + 2C_{12}(P) + 4C_{44}(P)}{2C_{11}(P) + 4C_{12}(P) - 4C_{44}(P)}, \quad (18)$$

where $C_{\alpha\beta}(P)$ is the pressure-dependent elastic constants for zinc-blende nitrides. In Eq. (17), $a_i(P)$ is the lattice constants which are dependent on P and can be given by [14]

$$a_i(p) = a_i(0)\left(1 - \frac{p}{3B_{0,i}}\right), \qquad i = 1,2, \quad (19)$$

where $B_{0,i}$ is the material dependent bulk modulus.

The pressure dependence of the electronic effective mass was given by[15]

$$\frac{m_{0,i}}{m_i(p)} = 1 + \frac{C_i}{E_{g,i}(p)}, \qquad i = 1,2, \quad (20)$$

where C_i is a fixed value for a given material with $P = 0$. The effective mass of $Al_xGa_{1-x}N$ can be obtained by the linear interpolation method. And $E_{{\rm g},i}(p) = E_{{\rm g},i}(0) + \alpha_{\rm i}p + \beta_{\rm i}p^2$ is the change of the energy gap with pressure[16]. The corresponding energy gap of a ternary mixed crystal (TMC) Al_xGa_{1-x} N can be determined by the SPCA[13]:

$$E_{\rm TMC} = \frac{E_{\rm A}E_{\rm B}}{xE_{\rm A} + (1-x)E_{\rm B}}. \quad (21)$$

For the pressure dependence of high frequency dielectric con-

Table 1. Parameters used in the computation.

Material	a (Å)	E_g (eV)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	ω_{LO} (cm^{-1})	ω_{TO} (cm^{-1})
GaN	4.50[a]	3.3[a]	287[b]	158[b]	159[b]	731[c]	551[c]
AlN	4.38[a]	4.9[a]	301[b]	166[b]	190[b]	908[c]	654[c]

[a] Ref. [18], [b] Ref. [19], [c] Ref. [20].

Table 2. Parameters used in the computation.

Material	α (meV/GPa)	β (meV/GPa^2)	κ_∞	f_i
GaN	39[d]	-0.32[d]	5.41[e]	0.5[g]
AlN	40[d]	-0.32[d]	4.46[f]	0.499[g]

[d]Ref. [16,] , [e] Ref. [21] , [f] Ref. [22] , [g]Ref. [23].

stant, we use the equation given by Goñi *et al* .[17]:

$$\frac{\partial \ln \kappa_\infty(P)}{\partial \ln V} \approx \frac{5\left[\kappa_\infty(P)-1\right]}{3\kappa_\infty(P)}(0.9-f_i), \tag{22}$$

where f_i is the ionicity of the material under pressure. The static dielectric constant κ_0 are derived from a generalized Lyddane-Sachs-Teller relation:

$$\kappa_0 = \kappa_\infty\left(\frac{\omega_{LO}}{\omega_{TO}}\right)^2, \tag{23}$$

where ω_{LO} and ω_{TO} are related to the frequencies of zone-center LO- and TO-phonons which can be determined by the given mode-Grüneisen parameters[10]:

$$\gamma_i = B_0\frac{1}{\omega_i}\frac{\partial\omega_i(P)}{\partial P}.$$

The dielectric constant of $Al_xGa_{1-x}N$ can be calculated by the SCPA[13]:

$$\kappa_{TMC} = [((1-x)m_B\kappa_A^2 + xm_A\kappa_B^2)(x/m_A + (1-x)/m_B)]^{1/2}. \tag{24}$$

The values of the mode-Grüneisen parameter γ are given in Table 1.

4. Result and discussion

We performed numerical computation for a strained zinc-blende GaN/$Al_xGa_{1-x}N$ heterojunctions. The parameters used in the computation are listed in Tables 1 and 2. The calculated results are shown by Figs. 1–6.

For a zinc-blende heterostructure, the band mass of the electron has been considered as isotropic: $m_\perp = m_{//}$. We only consider the pressure effect from 0 to 10 GPa and temperatures from 0 to 300 K.

In the strained heterojunction, for the given Al concentration $x = 0.3$, areal electronic density $n_s = 4.0\times10^{12}$ cm^{-2} and pressure P = 0, 4, 8 GPa, respectively, the relation between the polaronic self-trapping energies and temperature is given by Fig. 1. One can see clearly that the self-trapping energies E_s decrease gradually as the temperature increases. The change of energies can be observed only when $T > 85$ K, while the falling tendency become obvious at $T > 130$ K. The calculated result denotes that E_s decreases about 5.06% when $P = 0$ kbar and temperature changes from 100 to 300 K. It indicates that

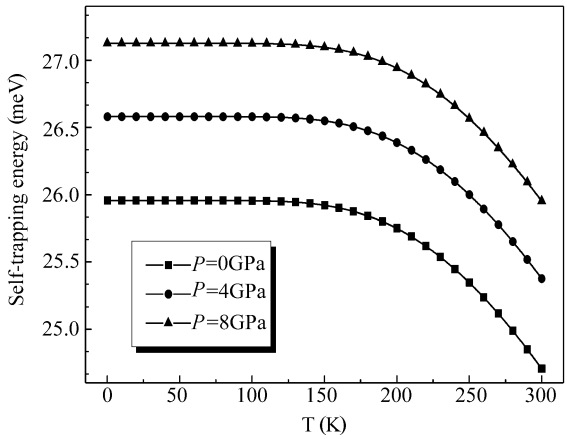

Fig. 1. Polaronic self-trapping energies in the strained zinc-blende GaN/$Al_xGa_{1-x}N$ heterojunction as functions of temperature under different pressures.

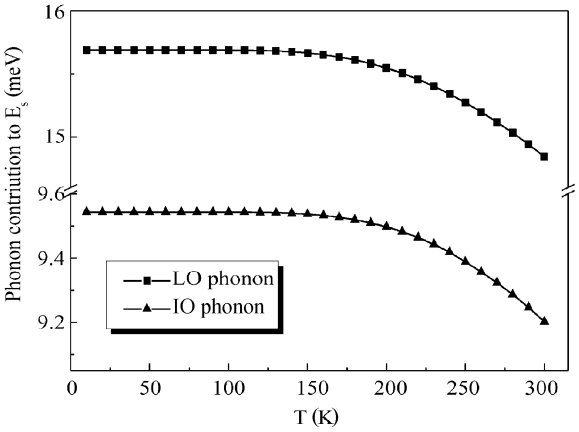

Fig. 2. Contribution to self-trapping energies from the LO phonons and IO phonon mode with higher frequency under zero pressure.

the average number of virtual phonon around an electron decreases obviously beyond some certain temperature. In other words, at this moment, the polaron loses its phonon clothing and becomes free-electron-like.

Figure 2 shows the contribution to E_s from the bulk LO phonons and the interface optical phonon mode with a higher frequency as functions of temperature under zero pressure. The calculated result denotes that E_s decreases very slowly when temperature changes from 100 to 200 K, whereas it shows a sharp decline tendency as the temperature continuously increases. It can be seen from the figure that both of them have the change tendency similar to that of E_s. When T ranges from 0 to 300 K, the net decrements of phonon contribution to E_s are 0.84, 0.35 meV with percentages of 5.68%, 3.71% for the bulk LO phonons and the higher frequency interface optical phonon, respectively. This fact shows that temperature

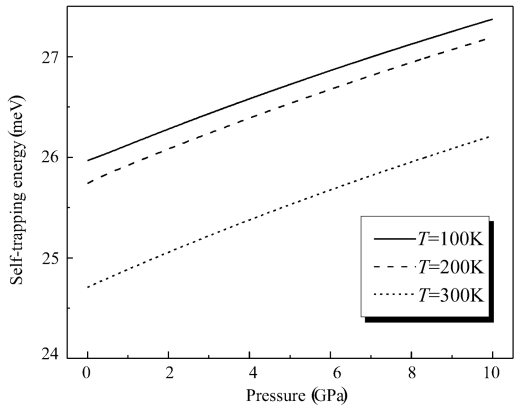

Fig. 3. Polaronic self-trapping energies in the strained zinc-blende GaN/Al_x Ga_{1-x}N heterojunction as functions of pressure at different temperatures.

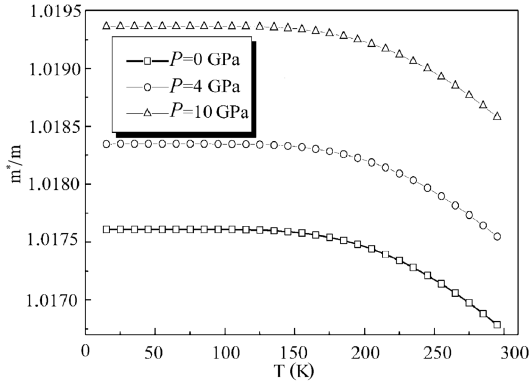

Fig. 4. Total effective mass in units of a bare electron mass m^* as functions the temperature T.

influence on the LO phonons is larger than on the interface optical phonon mode with a higher frequency. It was also found that the contribution from the IO phonon mode with a lower frequency is extremely small so that it can be neglected and the single IO mode approximation is good enough in the further discussion.

The results for E_s of a polaron in a free strained zinc-blende GaN/Al_xGa$_{1-x}$N heterojunction with the [111] orientation as functions of hydrostatic pressure are illustrated in Fig. 3 for areal electronic density $n_s = 4.0 \times 10^{12}$ cm^{-2}. It can be found that E_s increases near linearly with pressure, but shows a decrease trend as temperature increases. The calculated result denotes that E_s increases about 6.09% at $T = 300$ K and $P = 10$ GPa compared with that at $P = 0$ GPa. This is due to the competitive effect from pressure on physical parameters of material such as dielectric constants, phonon frequencies, electronic effective masses, barrier height, and conduction energy band bending, which induce a stronger two-dimensional property to strengthen the electron-phonon interaction. However, at a higher temperature, the average number of virtual phonons around an electron decreases to make the polaronic self-trapping "shallow". Furthermore, by our calculation it was also found that the contributions from the IO phonon modes with lower and higher frequencies also increase near linearly with pressure. Their tendency is similar to Fig. 3. The result has not been given here to shorten the pages.

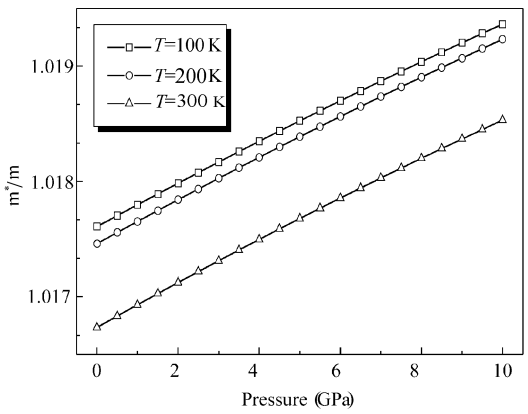

Fig. 5. Total effective mass in units of a bare electron mass m^* as functions of the hydrostatic pressure P.

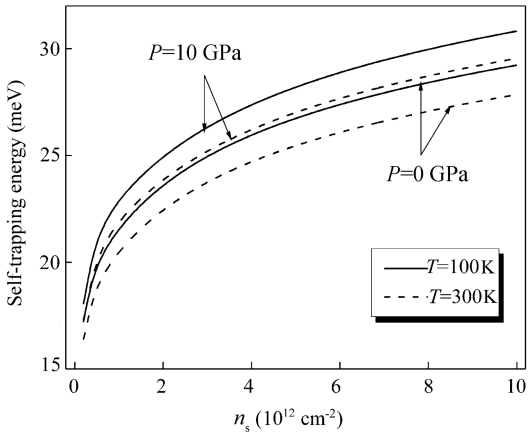

Fig. 6. Polaronic self-trapping energies as functions of areal electronic density for different pressures and temperatures.

It is shown in Fig. 4 that the total contributions to polaron effective masses from the three different phonon modes versus temperature for hydrostatic pressure $P = 0$, 4 and 10 GPa, respectively. The result indicates that the contributions from the LO phonons and IO phonon mode with a higher frequency decrease 6.7%, 4.58% for given $P = 4$ GPa as temperature changes from 0 to 300 K, whereas the contributions increase 9.12%, 20.7% at $T = 300$ K when pressure changes from 0 to 10 GPa. It is clearly seen that the pressure effect on effective mass is stronger than the temperature effect. It should be also pointed out that the influence from the IO phonon mode with a lower frequency is very small and can be neglected.

We plot in Fig. 5 the total contributions to the polaronic effective masses from the three different phonon modes versus hydrostatic pressure for $T = 100$, 200 and 300 K. One can see that effective masses of polarons increase near linearly with increasing of pressure. This property is similar to that of E_s .

In Fig. 6, we display E_s as a function of areal electronic density n_s varying with temperature and hydrostatic pressure. For a given interface potential and Al component, n_s strengthens the band bending and the 2D character of the polaron to increase E_s. The conduction band bending becomes stronger with increasing pressure to enforce the 2D property of electrons being more prominent. As a result, the bound energies increase gradually. It shows a decline trend with increasing

of temperature. This result is self-consistent with the results shown in previous figures.

5. Conclusions

Using a modified LLP variational method and a simplified coherent potential approximation on a strained zinc-blende nitride GaN/$Al_xGa_{1-x}N$ real heterojunction, we calculate the self-trapping energies and effective masses of interface polarons as functions of temperature, pressure and the areal electronic density. It shows that the polaronic self-trapping energies and effective masses increase near linearly with pressure when the modification of strain with hydrostatic pressure is considered whereas increase nonlinearly with the areal electronic density. Both of them are near constants at low temperature whereas decrease dramatically at high temperatures. The contributions from bulk LO phonon mode and one branch of IO phonon mode with a higher frequency are comparable important whereas the contribution from another branch of IO phonon mode with a lower frequency is small and can be neglected. The approximation of single IO mode can be adopted in future study.

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