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Effect of electron-phonon interaction on surface states in zinc-blende GaN, AlN, and InN under pressure

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Abstract. A variational approach is used to study the surface states of electrons in a semi-infinite polar semiconductor under hydrostatic pressure. The effective Hamiltonian and the surface-state levels are derived including the effects of electron-optical phonon interaction and pressure. The numerical computation has been performed for the surface-state energies versus pressure for zinc-blende GaN, AlN, and InN. The results show that the effect of electron-optical phonon interaction lowers the surface-state energy. It is also found that the effect of electron-surface optical phonon interaction is much bigger than the effect of electron-half space longitudinal optical phonon interaction for surface-state levels. It indicates that the surface-state energies and the influence of electron-phonon interaction increase with pressure obviously.

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1 Introduction

Among the III-V semiconductors, the wide band-gap nitrides GaN, AlN, and InN are currently actively investigated in view of their promising potential for optoelectronic applications in the blue to ultraviolet spectral range in recent years [1–5]. The vast majority of researches on the III-V nitrides have been focused on the wurtzite crystal phase. However, researchers have known for some time that the III-V nitrides also have zinc-blende phase [6]. The zinc-blende nitrides as a whole represent an unexplored material system whose properties may be quite different from those of their wurtzite counterparts. The zinc-blende nitrides may have superior electronic properties resulting from reduced phonon scattering in the higher symmetry crystal [7]. It is also hoped that the zinc-blended nitrides may be more amenable to *p*-type doping. Now that the capabilities to grow the zinc-blended nitrides have been demonstrated, a thorough investigation of the physical properties of these materials is timely.

The electronic surface-states in polar crystals have been widely studied by many experimental and theoretical scientists [8–12]. It is well-known that the termination of the lattice produces the intrinsic surface states, whose wave-functions are localized in the vicinity of the surface and decay rapidly inside the material [8–10]. However, the effects of electron-phonon (e-p) interactions on intrinsic surface states are rarely mentioned even though it is well-known that they influence considerably the properties of the electrons and give rise to polaron states in polar crystals [13–16]. In view of the imperfection of the nearly-free-electron approximation (NFEA) perturbation theory method [8], which becomes invalid when the band gap of the material is so broad that the perturbation can not be treated as a small disturbance. Recently, the authors used a variational theory to study the eigenvalue problems of the surface states of polarons in polar semiconductors, including both intrinsic surface electronic states and e-p interactions [11,12]. The results show that e-p interaction lowers the surface-state energy, and indicated that the surface optical (SO) phonon influence is dominant, especially for weak e-p coupling or narrow band gap materials. The pressure dependence of the physical properties in semiconductor bulk materials has been attracting considerable attention both experimentally and theoretically. The effect of pressure on the dielectric function of GaAs has been reported experimentally [17]. It is found that the high-frequency dielectric constant decrease with increasing pressure. Some authors studied the pressure properties of optical phonons [18], band-gap [19], effective mass [20,21] in bulk materials. Recently, pressure dependence of the dielectric and lattice-dynamical properties, optical phonon modes and transverse effective charges were investigated theoretically and experimentally in bulk

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GaN and AlN [2–4] and proved to be a valuable tool for deriving material parameters. These works impel farther investigations both in the bulk and surface structure materials. However, to our knowledge, the effect of hydrostatic pressure on the e-p interaction in the electronic surface states has not been reported. Therefore, theoretical investigations in detail for the effect of e-p interaction on the electronic surface states under pressure are invoked.

In this paper, we study the effects of e-p interaction on the electronic surface states for zinc-blende GaN, AlN, and InN under hydrostatic pressure, by using a variational treatment in the two-band model. Both of the effects of the discontinuity of lattices and the e-p interactions are considered, including electron-SO-phonon (e-SO-p) and electron-half space longitudinal optical (LO)-phonon (e-LO-p) interactions. An effective Hamiltonian for the surface states of electron in a semi-infinite polar crystals is obtained by using a Lee-Low-Pines (LLP)-like method [22] in Section 2. In Section 3, the pressure dependence of the parameter properties for zinc-blende GaN, AlN, and InN are investigated. A variational calculation for the surface-state energy of the polarons and the average penetrating depths of surface-state wave function are performed in Section 4 and the numerical results for nitrides semiconductors GaN, AlN, and InN are given and discussed in Section 5.

2 Effective Hamiltonian

Let us consider a semi-infinite polar crystal occupying the positive-half space $z \geq 0$, while the region $z < 0$ is a vacuum. An electron moving in the material will interact with the lattice vibrations. Using the NFEA and interactions between an electron and SO-phonon and half-space LO-phonon, the Hamiltonian of such an e-p system can be written as [8,11–14]

$$H = H_e + H_{ph} + H_{e-p}. \tag{1}$$

The first term in equation (1) is the electronic Hamiltonian and given by

$$H_e = \frac{p_t^2}{2m^*} + \frac{p_z^2}{2m_0} + V(z)\cdot \tag{2}$$

Here m^* is the band-mass of the electron in the $x-y$ plane. As a traditional treatment [8–10], the parabolic band approximation is adopted to describe the motion of electron in the plane since the translational symmetry is kept. m_0 is the rest mass of the electron and the 1D pseudo-potential $V(z)$ describing the potential experienced by the electron in the z-direction can be written as [8].

$$V(z) = \begin{cases} -2V_1 \cos(2\pi z/a), & z \geq 0 \\ V_0, & z \leq 0 \end{cases} \tag{3}$$

where V_0 and V_1 are respectively the vacuum energy level and half of the forbidden band gap (FEG) E_g in the two-band model. The second term is the free-phonon field Hamiltonian and has the well-known form

$$H_{ph} = \sum_k \hbar\omega_{\mathrm{LO}} a_k^+ a_k + \sum_q \hbar\omega_{\mathrm{SO}} b_q^+ b_q. \tag{4}$$

The third term in equation (1), e-p interactions term, can be written as

$$H_{e-p} = H_{e-\mathrm{LO}} + H_{e-\mathrm{SO}}, \tag{5}$$

where $H_{e-\mathrm{LO}}$ and $H_{e-\mathrm{SO}}$ stand for the Hamiltonians of the interactions between the electron and the half-space LO-phonon and SO-phonon, respectively, and can be given by

$$H_{e-\mathrm{LO}} = \sum_k \frac{1}{k} \sin(k_z z) \left(V_k^* e^{-i\vec{k}_t\cdot\vec{\rho}} a_k^+ + \mathrm{h.c.} \right), \tag{6a}$$

$$H_{e-\mathrm{SO}} = \sum_q \left(\frac{C^*}{q^{1/2}} e^{-q|z|} e^{-i\vec{q}\cdot\vec{\rho}} b_q^+ + \mathrm{h.c.} \right). \tag{6b}$$

In the equations, $\vec{r} = (\vec{\rho}, z)$, $\vec{p} = (\vec{p}_t, p_z)$, in which $\vec{\rho}$ and $\vec{p}_t$ are the $x-y$ plane components of the electron coordinates and momentum and z and p_z the z-component, respectively. $a_k^+(a_k)$ denotes the creation (annihilation) operator of a half-space LO-phonon with wave vector $\vec{k} = (\vec{k}_t, \vec{k}_z)$ and frequency ω_{LO}, while $b_q^+(b_q)$ the corresponding operator for a SO-phonon with 2D wave vector $\vec{q}$ and frequency ω_{SO}. V_k^* and C^* have been defined in reference [12].

To simplify the calculation for the effect of the e-p interactions, we first carry out two unitary transformations by using

$$U_1 = \exp\left[-i \sum_k a_k^+ a_k \vec{k}_t \cdot \vec{\rho} - i \sum_q b_q^+ b_q \vec{q} \cdot \vec{\rho} \right], \tag{7a}$$

and

$$U_2 = \exp\left[\sum_k \left(a_k^+ f_k - a_k f_k^* \right) + \sum_q \left(b_q^+ g_q - b_q g_q^* \right) \right]. \tag{7b}$$

Now let us consider a variational calculation to solve the Hamiltonian H. We will confine our discussion in the low-temperature limit and slow-motion electron case. Choosing an ansatz

$$|\psi\rangle = |\phi_\lambda(z)\rangle\,|0\rangle\,, \tag{8}$$

where the wave-vector $|0\rangle$ describes the zero-phonon state, $|\phi_\lambda(z)\rangle$ is the trial wave-function, whose variational parameter is λ. The total variational energy can be calculated by the following formulas

$$E = \left\langle \psi \left| U_2^{-1} U_1^{-1} H U_1 U_2 \right| \psi \right\rangle = \left\langle \phi_\lambda \left| H_f \right| \phi_\lambda \right\rangle, \tag{9}$$

where

$$H_f = \left\langle 0 \left| U_2^{-1} U_1^{-1} H U_1 U_2 \right| 0 \right\rangle, \tag{10}$$

the displacement amplitudes f_k and g_q in the unitary transformation (Eq. (7b)) can be determined by using a variational calculation similar to that used by LLP in bulk-polaron problems [11,22]. Miniming H_f as a function of $f_k(g_q)$ and $f_k^*(g_q^*)$ requires

$$\frac{\partial H_f}{\partial f_k^*} = 0, \qquad \frac{\partial H_f}{\partial g_q^*} = 0. \tag{11}$$

Using equations (10) and (11), we can obtain the effective polaron Hamiltonian H_f to be

$$H_f = \frac{P_t^2}{2m^{**}} + \frac{p_z^2}{2m_0} + V(z) + V_{eff}(z), \tag{12}$$

where V_{eff} is an effective potential in the direction of z

$$V_{eff}(z) = -\alpha_L \hbar\omega_{\rm LO}\eta(z) - \alpha_S\hbar\omega_{\rm SO}\beta(z) \tag{13}$$

with

$$\eta(z) = \frac{\pi}{2} - \int_0^\infty \frac{e^{-2u_L zR}}{1+R^2}dR, \quad \beta(z) = \int_0^\infty \frac{u_S e^{-2q|z|}dq}{q^2+u_S^2}, \tag{14a}$$

$$\alpha_L = \frac{m^* e^2}{\varepsilon\hbar u_L}, \qquad \alpha_S = \frac{m^* e^2}{\varepsilon^*\hbar^2 u_S}, \tag{14b}$$

$$u_L = \left(\frac{2m^*\omega_{\rm LO}}{\hbar}\right)^{1/2}, \qquad u_S = \left(\frac{2m^*\omega_{\rm SO}}{\hbar}\right)^{1/2}. \tag{14c}$$

Here α_L and α_S are respectively the coupling constants of the e-LO-p and e-SO-p interactions, H_f is a one-dimensional, two-band model Hamiltonian, which includes the e-p coupling and is called the effective polaron Hamiltonian. The SO-phonon frequency $\omega_{\rm SO}$ is given [14] as

$$\omega_{\rm SO} = \omega_{\rm TO}\left(\frac{\varepsilon_0+1}{\varepsilon_\infty+1}\right)^{1/2}\cdot \tag{15}$$

3 Pressure dependence of the parameter properties

In this section we present formalisms to studies lattice constant, dielectric function, optical phonon energy, band gap, and electronic band mass properties of zinc-blende nitrides semiconductors under hydrostatic pressure.

The pressure dependence of the lattice constant for bulk material can be obtained by expanding Murnaghan's equation state [23]

$$a(P) = a(0)\left(1 + P\frac{B'}{B}\right)^{-1/3B'}, \tag{16}$$

where B is the material bulk modulus and $B' = dB/dP$, in the low-pressure region, equation (16) reduces to

$$a(P) = a(0)\left(1 - P/3B\right)\cdot \tag{17}$$

Within the Penn gap model [24] and the dielectric theory of the covalent bond Phillips and Van Vechten [25,26] the high-frequency dielectric constant is given by

$$\varepsilon_\infty = 1 + DA\omega_p^2/\overline{E}_g^2 \qquad \text{with} \qquad \overline{E}_g^2 = E_h^2 + C^2. \tag{18}$$

Here, ω_p is the valence-electron plasma frequency and $\overline{E}_g$ is the average optical gap (or Penn gap), which spilt into a homopolar (covalent) contribution E_h and a ionic contribution C. The factor A is constant ($A \sim 1$) and $D = N_{eff}/4$ account for the effects of occupied d states on the interband transition probability. The plasma frequency varies as $\omega_p \sim V^{-1/2}$, and it is generally assumed that $dC/dP \approx 0$. The volume dependence of E_h and D is estimated to be $E_h \sim V^{0.83}$ and $D - 1 \sim V^{4.3}$ (Refs. [25,26]). The volume derivative of ε_∞ can be than written in terms of the Phillps-Van Vechten ionicity $f_i = C^2/E_g^2$ as [26]

$$\frac{\partial \ln\varepsilon_\infty}{\partial \ln V} \approx \frac{5(\varepsilon_\infty - 1)}{3\varepsilon_\infty}(0.9 - f_i)\cdot \tag{19}$$

The pressure dependence of the volume can be written as $\partial P/\partial V = -B/V$. One can obtain the dielectric constant the following form

$$\varepsilon_\infty(P) = 1 + \left[\varepsilon_\infty(0) - 1\right] e^{-\frac{5}{3B}(0.9-f_i)P}. \tag{20}$$

According to equation (19) the borderline between a "covalent" and "ionic" pressure dependence of ε_∞ is given by $f_i \approx 0.9$.

In order to obtain the effect of hydrostatic pressure of the e-p interaction coupling strength in surface structure systems, we need to know the pressure dependence of the bulk optical phonon energy. To do so, we examine the mode-Grüneisen parameter under the low-pressure

$$\gamma_j = -\left.\frac{\partial\ln\omega_j}{\partial\ln V}\right|_{V=V_0} = B\left.\frac{\partial\omega_j}{\partial P}\right|_{P=0}, \quad j = L, T \tag{21}$$

for a phonon mode j with the frequency. $j = L, T$ label the LO- and TO-phonons respectively. Since γ_j is nearly constants in low-pressure for bulk LO- and TO-phonons respectively, the modification of phonon energy due to pressure can be expressed as

$$\hbar\omega_j(P) = \hbar\omega_j(0)e^{\frac{\gamma_j}{B}P}. \tag{22}$$

The "0" subscript denotes that quantities are evaluated at $P = 0$. Equation (22) shows that the phonon frequency increase as the pressure increasing. It may be seen that the result agrees with calculation of the self-consistent density-functional perturbation theory [27].

To obtain the pressure effect on the surface-state energies of the polarons for the zinc-blende nitrides GaN, AlN and InN materials, we need the information about the variation of band-gap and electronic band masses with pressure. At low pressure, one can fit the band-gap $E_g(P)$ to a quadratic function [19]

$$E_g(P) = E_g(0) + bP + cP^2. \tag{23}$$

Table 1. Parameters used in the calculation (room temperature and zero external pressure). Energy is measured in meV and mass in electron rest mass m_0.

Materials	a(nm)	E_g	$\hbar\omega_{\text{LO}}$	$\hbar\omega_{\text{TO}}$	ε_0	ε_∞	m^*	B(GPa)	γ_{LO}	γ_{TO}	f_i
GaN	0.452 [2]	3300 [2]	92.96 [28]	69.41 [28]	9.6 [28]	5.35 [28]	0.15 [29]	201 [29]	1.2 [4]	1.4 [4]	0.5 [26]
AlN	0.433 [2]	5110 [2]	112.46 [28]	82.05 [28]	9.08 [28]	4.84 [28]	0.25 [29]	203 [29]	1.06 [4]	1.41 [4]	0.449 [26]
InN	0.498 [2]	2200 [2]	73.87 [28]	57.88 [28]	13.6 [28]	8.4 [28]	0.12 [29]	139 [29]	1.08 [30]	1.5 [30]	0.578 [26]

Adopting the data of reference [19], we obtain the values $b = 35.88$ meV/GPa, $c = -0.804$ meV/GPa^2 for GaN, $b = 5.24$ meV/GPa, $c = -0.102$ meV/GPa^2 for AlN (indirect band gap), and $b = 24.73$ meV/GPa, $c = -0.785$ meV/GPa^2 for InN. The pressure dependence of the electronic band mass can be expressed as follow [20,21]

$$\frac{m_0}{m^*} \approx 1 + \frac{2\hbar^2}{m_0 a^2}\frac{1}{\overline{E}_g}, \tag{24}$$

where $\overline{E}_g$ is the average gap of the bulk material discussed. Equation (18) can also be rewritten as

$$\frac{m_0}{m^*(P)} = 1 + \frac{A}{E_g(P)}\cdot \tag{25}$$

In terms of the electronic band masses of the material GaN, AlN and InN at zero external pressure (seen Tab. 1), we can find the values $A = 13.2$ eV (GaN), 15.3 eV (AlN) and 16.1 eV (InN), respectively.

4 Variational energy

At this juncture, we use the effective Hamiltonian of equation (12) to solve the surface-state polaron problems. In the following, we can set $P_t = 0$ without loss of generality because we are concerned with only the surface state and the electron transverse motion is unimportant. Therefore the effective Hamiltonian H_f of a surface-state polaron in a semi-infinite polar crystal can simplifies to

$$H_{\mathit{eff}} = \frac{p_z^2}{2m_0} + V(z) + V_{\mathit{eff}}(z), \tag{26}$$

the corresponding variational energy being given by

$$E_V = \langle\phi_\lambda(z)\,|H_{\mathit{eff}}|\,\phi_\lambda(z)\rangle \tag{27}$$

where $|\phi_\lambda(z)\rangle$ has been pointed as a trial wave-function and can be chosen as [8,11,12]

$$|\phi_\lambda(z)\rangle = \begin{cases} Ae^{-\lambda_1 z}\cos(\pi z/a + \lambda_2), & z \geq 0 \\ Be^{qz}, & z \leq 0 \end{cases} \tag{28}$$

with a being the lattice constant of the polar crystal. The surface of the material has been assumed to lie at exactly the center of an atom [8], and treat λ_1 and λ_2 as variational parameters to seek the surface-state energy by a variational calculation. Matching $\phi_\lambda(z)$ and $\phi'_\lambda(z)/\phi_\lambda(z)$ at $z = 0$, provides the relationships:

$$A\cos\lambda_2 = B, \tag{29a}$$

$$q = -\left(\lambda_1 + \frac{\pi}{a}\tan\lambda_2\right), \tag{29b}$$

while one of the normalization constants A is determined by

$$A^{-2} = -\frac{\cos^2\lambda_2}{2\left(\lambda_1 + \dfrac{\pi}{a}\tan\lambda_2\right)} + \frac{1}{4}\left(\frac{\lambda_1\cos 2\lambda_2 - \dfrac{\pi}{a}\sin 2\lambda_2}{\lambda_1^2 + \pi^2/a^2} + \frac{1}{\lambda_1}\right)\cdot \tag{30}$$

The surface-state variational energy then can be written as

$$E_V = E_e - E_{e-\text{LO}} - E_{e-\text{SO}}, \tag{31}$$

where

$$\begin{aligned} E_e =& \frac{\pi^2\hbar^2 A^2}{8m_0 a^2\lambda_1} - \frac{V_0}{2}\frac{A^2\cos\lambda_2}{\lambda_1 + \dfrac{\pi}{a}\tan\lambda_2} \\ &- \frac{V_1 A^2}{4}\left(\frac{\cos 2\lambda_2}{\lambda_1} + \frac{2\lambda_1}{\lambda_1^2 + \pi^2/a^2}\right. \\ &\left.+ \frac{\lambda_1\cos 2\lambda_2 - \frac{2\pi}{a}\sin 2\lambda_2}{\lambda_1^2 + 4\pi^2/a^2}\right), \end{aligned} \tag{32a}$$

$$E_{e-\text{LO}} = \alpha_L\hbar\omega_{\text{LO}}\left[\frac{\pi}{2} - A^2\left(g_1 + g_2\cos^2\lambda_2\right)\right], \tag{32b}$$

$$E_{e-\text{SO}} = \alpha_S\hbar\omega_{\text{SO}}A^2\left(I_1 + I_2\cos^2\lambda_2\right), \tag{32c}$$

with

$$g_1 = \int_0^\infty \frac{1}{4(1+k^2)}\left[\frac{1}{\lambda_1 + u_L k} + \frac{(\lambda_1 + u_L k)\cos 2\lambda_2 - \frac{\pi}{a}\sin 2\lambda_2}{(\lambda_1 + u_L k)^2 + \pi^2/a^2}\right]dk,$$

$$g_2 = -\int_0^\infty \frac{dk}{2\left(1+k^2\right)\left(\lambda_1 + \frac{\pi}{a}\tan\lambda_2 - u_L k\right)},$$

and

$$I_1 = \int_0^\infty \frac{u_S}{4(q^2+u_S^2)}\left[\frac{1}{\lambda_1+q} + \frac{(\lambda_1+q)\cos 2\lambda_2 - \frac{\pi}{a}\sin 2\lambda_2}{(\lambda_1+q)^2+\pi^2/a^2}\right]dq,$$

$$I_2 = -\int_0^\infty \frac{u_S dq}{2\left(q^2+u_S^2\right)\left(\lambda_1+\frac{\pi}{a}\tan\lambda_2 - q\right)}.$$

The average penetrating depth of surface state wave function is given by

$$d = \langle\phi_\lambda\,|z|\,\phi_\lambda\rangle \qquad z \geq 0$$
$$= \frac{A^2}{8}\left[\frac{1}{\lambda_1^2} + \frac{\left(\lambda_1^2-\pi^2/a^2\right)\cos 2\lambda_2 - 2\lambda_1\frac{\pi}{a}\sin 2\lambda_2}{\left(\lambda_1^2+\pi^2/a^2\right)^2}\right]. \tag{33}$$

The variational parameters λ_1 and λ_2 can be determined by the equation

$$\partial E_V/\partial\lambda_i = 0, \qquad i = 1,\,2. \tag{34}$$

The complexity of equation (34) gives rise to the need for numerical solutions. Using equations (31–34), we can obtain the average penetrating death of surface-state wave function d and the minimum of the variational energy E_V, *i.e.* the surface-state energy E_S.

In equation (31) $E_{e-\mathrm{LO}}$ and $E_{e-\mathrm{SO}}$ correspond to respectively the e-LO-p and e-SO-p interactions contributions.

5 Numerical results and discussion

We have numerically computed the surface-state energies of the polarons for zinc-blende nitrides GaN, AlN, and InN. For the sake of comparison we have also calculated the surface-state energies of the electron without including the e-p interactions. The parameters used in the computations are listed in Table 1 and the results are illustrated in Figures 1–3.

To clearly understand the effects of the e-p interaction on the surface states, we have plotted in Figure 1 the surface-state levels with and without the phonons influences as functions of the hydrostatic pressure P for the materials GaN, AlN, and InN, here we put the surface potential to be a reasonable value $V_0 = 5.0$ eV [8] in the computations for reference. For ease of presentation, we have chosen the values of the pressure P to vary in the reasonable range 0–30 GPa [3,4] in the numerical computations. It is clearly seen from Figure 1 that the pressure raised the surface-state levels obviously for all the computed materials. There is nearly linear increase from the zero-pressure values with rising pressure, where linear terms are about 4.0 meV/GPa, 5.4 meV/GPa, and 4.2 meV/GPa corresponding to GaN, AlN and InN, respectively. Comparing the result at P = 30 GPa with that at P = 0 GPa, we found that the net increases are 120.9 meV, 160.7 meV, and 122.0 meV for GaN, AlN and InN, respectively. This is due to the competition of change among the lattice constant a and the band-gap E_g with pressure. The direct effect of the pressure is to decrease the lattice constant a, and to increase the band-gap E_g. On the other band, the electron effective mass and the optical phonon frequency increase with pressure, but the dielectric constant decrease with pressure. It makes the pressure effect more complicated.

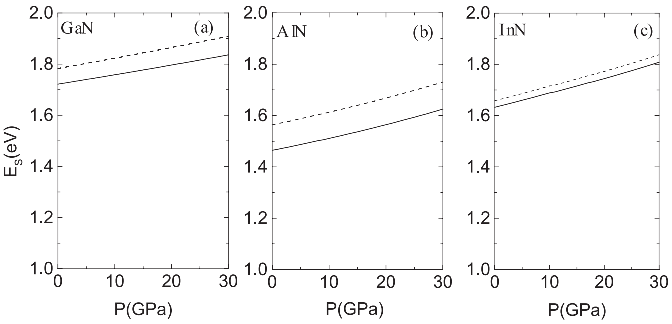

Fig. 1. The surface-state levels E_S with (solid line) without (dashed line) e-p interactions as function of the pressure P for: (a) GaN, (b) AlN and (c) InN.

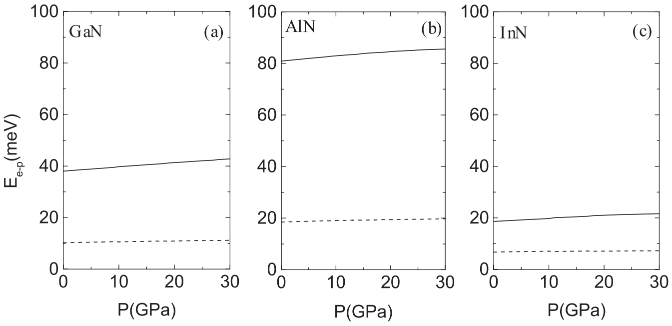

Fig. 2. The surface-state energy shifts $E_{e-\mathrm{SO}}$ (solid line) and $E_{e-\mathrm{LO}}$ (dashed line) by e-p interactions as functions of the pressure P for: (a) GaN, (b) AlN and (c) InN.

As is expected that the electronic surface states including the e-p interaction are always lower than that without including the phonon effects for all the computed materials. In other words, the e-p interaction lowers the levels of the surface states. It is also found in Figure 1 that the two curves of the surface-state levels with and without the phonon effects are separated by about scores of meV. It is also seen that the effect of e-p interaction on surface states is obvious. The curves for the materials GaN and AlN in Figure 1a and Figure 1b are separated more distinctly from each other than the material InN does. On the other hand, the surface-state levels shifts are also related to the width of the band-gap E_g. It follows that the stronger e-p coupling or broader width E_g is, the greater the shift of surface-state energy. Furthermore, these results and those of our previous works [11,12] for the phonon effects are

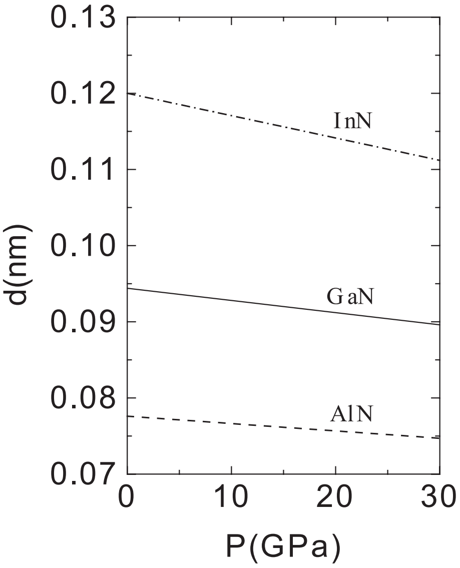

Fig. 3. The average penetrating depths d of surface state wave function as functions of the pressure P.

almost alike, but the phonon influences are more obvious for the wide band-gap semiconductors GaN, AlN and InN. This can be seen from Figure 2.

In Figure 2, we have illustrated the shifts $E_{e-\mathrm{SO}}$ and $E_{e-\mathrm{LO}}$ of surface-state energies by the interactions between the electron and the half-space LO-phonon and SO-phonon as functions of the hydrostatic pressure P for the above materials with $V_0 = 5.0$ eV. It is clearly seen that the half-space LO-phonon effect is less value than SO-phonon effect for the energy levels of the surface states. It follows that the stronger the e-p coupling, the greater are the half-space LO-phonon and SO-phonon influences, respectively. These shifts are at zero-pressure $E_{e-\mathrm{SO}} = 38.04$ meV and $E_{e-\mathrm{LO}} = 10.24$ meV for GaN, $E_{e-\mathrm{SO}} = 80.90$ meV and $E_{e-\mathrm{LO}} = 18.46$ meV for AlN, and $E_{e-\mathrm{SO}} = 19.54$ meV and $E_{e-\mathrm{LO}} = 6.12$ meV for InN, respectively. It is also found that these shifts are slow linear increases with pressure. Comparing the result at $P =$ 30 GPa with that at $P = 0$ GPa, we found that $E_{e-\mathrm{SO}}$ and $E_{e-\mathrm{LO}}$ increase to 12.5% and 9.3%, whereas the net increases are 4.76 meV($E_{e-\mathrm{SO}}$) and 0.96 meV($E_{e-\mathrm{LO}}$) respectively for GaN. Meanwhile, AlN and InN correspond closely to GaN in Figure 2. It is shown that the contributions from SO-phonon and half-space LO-phonon are different. The SO-phonon contribution is dominant, especially for materials with stronger e-p couplings or broad band gap material AlN, but half-space LO-phonon contribution cannot be also neglected, even if weak e-p coupling or narrow band gap material InN. It is indicated that the pressure dependence of the SO-phonon influence on surface states is more obvious than the half-space LO-phonon does, and the half-space LO-phonon influence is small with pressure.

The average penetrating depth, between the electronic surface states and the material surface, are plotted as functions of the hydrostatic pressure P in Figure 3 for the aforesaid materials with $V_0 = 5.0$ eV. It can be seen that the average penetrating depths d are only about 0.1 nm, so it is less than the lattice constant of the aforesaid materials. It shows that the electronic surface states are localized near the surface [8], hence effect of e-SO-p interaction on the surface-state of electron is dominant. It is also found that the average penetrating depths d decrease as the pressure increase for the all materials. The pressure makes the electron to move near surface, and raises the electronic surface-state energies.

In summary, we have investigated the pressure effect of the surface states of an electron in zinc-blend nitrides semiconductors including e-p interaction by a variational treatment. The energy level of a surface-state polaron has been calculated. The effects of the e-p interaction on the surface states are obtained and discussed under hydrostatic pressure for GaN, AlN, and InN materials. The numerical results show that the e-p coupling lowers the surface-state energy levels, so the phonon and pressure effects is obvious. It is also found that the SO-phonon influence on the surface-state of electron is dominant. It indicates that the surface-state energies and the influence of e-p interaction increase with pressure obviously.

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References

1. S. Nakamura, *The Blue Laser Diode-GaN Based Light Emitters and Lasers* (Springer, Berlin, 1997)
2. S. Strite, H. Morkoc, J. Vac. Sci. Technol. B **10**, 1237 (1992)
3. J.-M. Wagner, F. Bechstedt, Phys. Rev. B **62**, 4526 (2000)
4. A.R. Goñi, H. Siegle, K. Syassen, C. Thomsen, J.-M. Wagner, Phys. Rev. B **64**, 035205 (2001)
5. P. Perlin, T. Suski, J.W. Ager III, G. Conti, A. Plian, N.E. Christensen, I. Gorczyca, I. Grzegory, E.R. Weber, E.E. Haller, Phys. Rev. B **60**, 1480 (1999)
6. W. Seifert, A. Tempel, Phys. Status Solidi (a) **23**, K39 (1974); M. Mizuta, S. Fujieda, Y. Matsumoto, T. Kawamura, Jpn J. Appl. Phys. **25**, L945 (1986)
7. W.R.L. Lambrecht, B. Segall, Phys. Rev. B **43**, 7070 (1991); P. Das, D.K. Ferry, Solid State Electron. **19**, 851(1976)
8. S.G. Davison, M. Steslicka, *Basic Theory of Surface States* (Clarendon Press, Oxford, 1992), Chap. 5
9. F. Garcia-Moliner, F. Flores, J. Phys. C **9**, 1609 (1976)
10. J.B. Pantry, S.J. Gurman, Surf. Sci. **49**, 87 (1975)
11. X.X. Liang, Z.W. Yan, Surf. Sci. **400**, 232 (1998)
12. Z.W. Yan, X.X. Liang, Solid State Commun. **110**, 451 (1999); Eur. Phys. J. B **15**, 531 (2000)
13. E. Evans, D.L. Mills, Phys. Rev. B **8**, 4004 (1973)
14. N. Mori, T. Ando, Phys. Rev. B **40**, 6175 (1989)
15. X.X. Liang, S.G. Davison, Surface Science, **298**, 225 (1993)
16. F.M. Peeters, J.T. Devreese, Phys. Rev. B **36**, 4442 (1987)

17. A.R. Goñi, K. Syassen, M. Cardona, Phys. Rev. B **41**, 10104 (1990)
18. M. Holtz, M. Seon, O. Brafman, R. Manor, D. Fekete, Phys. Rev. B **54**, 8714 (1996)
19. S.H. Wei, A. Zunger, Phys. Rev. B **60**, 5404 (1999)
20. P. Lefebvre, B. Gil, H. Mathieu, Phys. Rev. B **35**, 5630 (1987)
21. B. Sukumar, K. Navaneethakrishana, Phys. Status Solidi (b) **158**, 193 (1990)
22. T.D. Lee, F.E. Low, D.Pines, Phys. Rev. **90**, 297 (1953)
23. J.A. Tuchman, S. Kim, Z. Sui, I.P. Herman, Phys. Rev. B **46**, 13371 (1992)
24. D.R. Penn, Phys. Rev. **128**, 2093 (1962)
25. J.A. Van Vechten, Phys. Rev. **182**, 891 (1969)
26. J.C. Phillips, *Bonds and Bands in Semiconductors* (Academic Press, 1973)
27. P. Giannozzi, S. De Gironcoli, P. Pavone, S. Baroni, Phys. Rev. B **45**, 10123 (1992)
28. C. Bungaro, K. Rapcewicz, J. Bernholc, Phys. Rev. B **61**, 6720 (2000)
29. I. Vurgaftman, I.R. Ram-Mohan, J. Appl. Phys. **89**, 5815 (2001)
30. K. Kim, W.R.L. Lambrecht, B. Segall, Phys. Rev. B **53**, 16310 (1996)