Energy of a Polaron in a Wurtzite Nitride Finite Parabolic Quantum Well *

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The effects of electron–phonon interaction on energy levels of a polaron in a wurtzite nitride finite parabolic quantum well (PQW) are studied by using a modified Lee–Low–Pines variational method. The ground state, first excited state, and transition energy of the polaron in the $GaN/Al_{0.3}Ga_{0.7}N$ wurtzite PQW are calculated by taking account of the influence of confined LO(TO)-like phonon modes and the half-space LO(TO)-like phonon modes and considering the anisotropy of all kinds of phonon modes. The numerical results are given and discussed. The results show that the electron–phonon interaction strongly affects the energy levels of the polaron, and the contributions from phonons to the energy of a polaron in a wurtzite nitride PQW are greater than that in an AlGaAs PQW. This indicates that the electron–phonon interaction in a wurtzite nitride PQW is not negligible.

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In recent years, the semiconductor materials GaN, AlN and InN, together with the compounds AlGaN and InGaN and their heterostructures, have become important in several photonic and electronic applications. Examples include light emitters covering the UV and visible range, and high temperature and high power microwave electronics. The basis for these applications is the large direct band gap of GaN. Moreover, the mismatches in lattice constant and the strain have been exploited and developed to realize new structures, such as quantum wires and quantum dots. Very recently, Gurusinghe *et al.*[1] analysed electron scattering from phonons, ionized impurities, line dislocations, and interface roughness at $GaN/Al_xGa_{1-x}N$ interface. They found that these mechanisms are responsible for mobility limitations in a two-dimensional electron gas. At temperatures below 50 K, ionized impurity scattering and line dislocation scattering were found to limit the mobility. For temperatures at and above room temperature, optical phonon scattering would be predominant.

It has been shown that the Ⅲ-Ⅴ nitrides have a wurtzite phase and a zinc-blende phase.[2−8] The zinc-blende structures have superior electronic properties resulting from their higher symmetry. However, since wurtzite crystals have a different unit-cell structure and lower symmetry compared to their zinc-blende counterparts, they have many more distinct phonon branches and phonon modes. The optical-phonon branches support mixed longitudinal and transverse modes due to the anisotropy of wurtzite crystal. Researchers have presented the Fröhhich-like electron–optical phonon interaction Hamiltonians in bulk GaN and wurtzite heterostructure based on the macroscopic dielectric continuum model and the uniaxial model.[2−4] Furthermore, they analysed in detail the dependence of scattering rate on optical anisotropy and dimensionally induced transformation of the phonon spectra. The polaron effect has also been studied in wurtzite nitride crystal by some authors.[7,8] The result that structure anisotropy increases the electron–phonon interaction in wurtzite nitride semiconductors appears to be universal.

Meanwhile, rapid progress in crystal growth and microfabrication technologies has allowed us to explore the properties of unusual nanometre-scale semiconductor structures, such as parabolic quantum wells (PQWs)[9] and triangular quantum wells (TQWs).[10] The different properties of PQWs from square quantum wells (SQWs) have attracted much attention of many experimental and theoretical physicists in recent years.[11−19] A series of equally spaced resonant current peaks related to the sub-band levels of confined electrons were observed in the experiments by Capasso *et al.*[11] Further, Bechstedt *et al.*[12] investigated the two-mode behaviour of optical phonons within a random-element-isodisplacement model and showed that the composition profile in fabricated quantum wells can remarkably influence the properties of phonons and the electron–phonon (e-p) interaction. Very recently, LO-phonon assisted tunnelling through a PQW with double barriers has been studied,[16] and it was found that the LO-phonons play an important role in electron tunnelling. The donor and exciton states as well as the polaronic effects in PQWs have also been studied and compared to the situation in

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SQWs.[13,14] However, few works on the polaron problem in wurtzite PQWs have been reported. Further investigation of wurtzite PQWs will help us understand the properties of wurtzite nitride semiconductors.

In this Letter, we report our study of the polaron energy in a wurtzite nitride finite PQW by considering structure anisotropy. We consider the confined slab LO(TO)-like phonon modes and the half-space LO(TO)-like phonon modes in our calculation. The ground state energy, first excited state energy, and transition energy from the ground state to the first excited state with the phonon effect are obtained using a modified Lee–Low–Pine (LLP) method.

We consider a PQW structure of polar dielectrics for which the well material is in a region $\lambda = 1$, $|z| = d$, and the barriers are in a region $\lambda = 2$, $|z| > d$. The well material is generated by alternating multiple layers of GaN and $Al_{0.3}Ga_{0.7}N$ of varying thickness along the z direction. The relative thickness of the GaN layers in the PQW increases quadratically with increasing distance from the well centre ($z = 0$), while that of the $Al_{0.3}Ga_{0.7}N$ layers decreases.[9] The barrier materials all are $Al_{0.3}Ga_{0.7}N$. An electron travels in the system, and couples with the LO(TO)-like phonon modes. Using the effective-mass approximation, the Hamiltonian of the electron–phonon system can be written as

$$H = \frac{p^2}{2m_{b\lambda}} + V(z) + \sum_{\boldsymbol{w}\lambda p} \hbar\omega_\lambda a_\lambda^+(\boldsymbol{w}) a_\lambda(\boldsymbol{w}) + H_l, \tag{1}$$

where the first term is the kinetic energy of the electron; $m_{b\lambda}$ is the effective-band mass of the electron in region λ; $a_\lambda^+(\boldsymbol{w})$ and $a_\lambda(\boldsymbol{w})$ are, respectively, the creation and annihilation operators for an LO (or TO) phonon with frequency ω, wave vector $\boldsymbol{w} = (\boldsymbol{q}, k_{\lambda z})$ and parity p with $\boldsymbol{q}$ being the two-dimensional wave vector. The second term is the parabolic well potential experienced by the electron, which can be written as

$$V(z) = \begin{cases} V_0 z^2/d^2 & |z| \le d, \\ V_0 & |z| > d. \end{cases} \tag{2}$$

Here $V_0 = 436.8\,\mathrm{meV}$[20] is the depth of the PQW.

The last term in Eq. (1) is the Hamiltonian of the interaction between the electron and the LO(TO)-like phonon modes and is given by[3]

$$H_I = \sum_{\boldsymbol{w}\lambda p} [g_p e^{-i\boldsymbol{q}\cdot\boldsymbol{\rho}} a_\lambda^+(\boldsymbol{w}) + \mathrm{H.c.}]. \tag{3}$$

The coupling function g_p in Eq. (3) is determined by

$$g_s = -\{4\pi\hbar e^2 L_1^{-2} \cdot [(\partial/\partial\omega)(\varepsilon_{1\perp}(\omega)q^2 + \varepsilon_{1z}(\omega)k_{1m}^2)d - 2q(\partial/\partial\omega) f_s(\omega) \cdot \cos(k_{1m}d)]^{-1}\}^{1/2} T_1, \tag{4}$$

with

$$T_1 = \begin{cases} \cos(k_{1m}z) & |z| \le d, \\ \cos(k_{1m}d) e^{-\kappa_2(|z|-d)} & |z| > d, \end{cases}$$

for symmetric confined modes; and

$$g_A = -\{4\pi\hbar e^2 L_1^{-2}[(\partial/\partial\omega)(\varepsilon_{1\perp}(\omega)q^2 + \varepsilon_{1z}(\omega)k_{1m}^2)d - 2q(\partial/\partial\omega) f_a(\omega) \cdot \sin(k_{1m}d)]^{-1}\}^{1/2} T_2, \tag{5}$$

with

$$T_2 = \begin{cases} \sin(k_{1m}z) & |z| \le d, \\ \mathrm{sgn}\,(z)\sin(k_{1m}d) e^{-\kappa_2(|z|-d)} & |z| > d, \end{cases}$$

for antisymmetric confined modes;

$$g_s = \Big[\frac{4\pi e^2\hbar L_1^{-3}}{(\partial/\partial\omega)(\varepsilon_{2\perp}\sin^2\theta_2 + \varepsilon_{2z}\cos^2\theta_2)}\Big]^{1/2} \cdot \frac{\sqrt{2}}{\sqrt{q^2 + k_{2z}^2}} [\varepsilon_{1z}^2 k_1^2 \sinh^2(k_1 d) + \varepsilon_{2z}^2 k_{2z}^2 \cosh^2(k_1 d)]^{-1/2} T_3, \tag{6}$$

with

$$T_3 = \begin{cases} \varepsilon_{1z}k_1 \sinh(k_1 d)\sin[k_{2z}(|z| - d)] \\ \quad + \varepsilon_{2z}k_{2z}\cosh(k_1 d) \\ \quad \cdot \cos[k_{2z}(|z| - d)], & |z| > d, \\ \varepsilon_{2z}k_{2z}\cosh(k_1 z) & |z| < d, \end{cases}$$

for symmetric half-space modes; and

$$g_A = \Big[\frac{4\pi e^2\hbar L_1^{-3}}{(\partial/\partial\omega)(\varepsilon_{2\perp}\sin^2\theta_2 + \varepsilon_{2z}\cos^2\theta_2)}\Big]^{1/2} \cdot \frac{\sqrt{2}}{\sqrt{q^2 + k_{2z}^2}} [\varepsilon_{1z}^2 k_1^2 \cosh^2(k_1 d) + \varepsilon_{2z}^2 k_{2z}^2 \sinh^2(k_1 d)]^{-1/2} T_4, \tag{7}$$

with

$$T_4 = \begin{cases} \mathrm{sgn}(z)\{\varepsilon_{1z}k_1 \cosh(k_1 d) \\ \quad \cdot \sin[k_{2z}(|z| - d)] + \varepsilon_{2z}k_{2z}\sinh(k_1 d) \\ \quad \cdot \cos[k_{2z}(|z| - d)]\}, & |z| > d, \\ \varepsilon_{2z}k_{2z}\sinh(k_1 z), & |z| < d/2, \end{cases}$$

for antisymmetric half-space modes.

Here L_1^2 is the cross-sectional area of the sample and $r = (\rho^2 + z^2)^{1/2}$ is the coordinate of electron. The definition of $\varepsilon_{\lambda\perp}(\omega)$, $\varepsilon_{\lambda z}(\omega)$, k_{1m}, κ_2, $f_s(\omega)$, $f_a(\omega)$, κ_1, θ_2, and k_{2z} can be found in Ref. [3].

The Hamiltonian in Eq. (1) is too complicated to be solved exactly. We now perform two unitary transformations with

$$U_1 = \exp\Big[-i\Big(\sum_{\boldsymbol{w}\lambda p} \boldsymbol{q}\cdot\boldsymbol{\rho} a_\lambda^+(\boldsymbol{w}) a_\lambda(\boldsymbol{w})\Big]\Big], \tag{8}$$

$$U_2 = \exp\Big\{\sum_{\boldsymbol{w}\lambda p}[h_\lambda a_\lambda^+(\boldsymbol{w}) - h_\lambda^* a_\lambda(\boldsymbol{w})]\Big\}. \quad (9)$$

The transformed Hamiltonian is given by

$$H^* = U_2^{-1}U_1^{-1}HU_1U_2. \quad (10)$$

Here the displacement amplitude h_λ and h_λ^* are a variational parameters that will be determined by minimizing the energies of the electron- phonon system. The wave function of the polaron can be expressed in the form

$$\psi_n = N_n\phi_n(z)|0\rangle, \quad (11)$$

where N_n is the normalization constant, $|0\rangle$ is the zero-phonon state of the phonon field, and $\phi_n(z)$ is the wave function in the z direction. The polaron energy can then be written as

$$E_n(h_\lambda, L) = \langle\psi_n|H^*|\psi_n\rangle. \quad (12)$$

For the ground state,[21]

$$\phi_1(z) = \begin{cases} F\left(\alpha, \frac{1}{2}, z^2/\beta d^2\right)\exp(-z^2/(2\beta d)^2) & \\ & |z| \le d, \\ B\exp(-\gamma z/d), & |z| > d, \end{cases} \quad (13)$$

and the first excited state,[21]

$$\phi_2(z) = \begin{cases} F\left(\alpha+\frac{1}{2}, \frac{3}{2}, z^2/\beta d^2\right)\exp(-z^2/(2\beta d)^2) & \\ & |z| \le d, \\ B_1 z\exp(-\gamma z/d), & |z| > d. \end{cases} \quad (14)$$

The definitions of the parameters (α, β, γ) in Eq. (13) are given in Ref. [21]. Substituting Eqs. (11), (13) and (14) into Eq. (12), one can obtain the ground state energy E_1 and the first excited state energy E_2 of the polaron. The transition energy from the ground state to the first excited state can be given by

$$\Delta E = E_2 - E_1. \quad (15)$$

For comparison we have also calculated the ground state energy of a polaron in the SQW. The energies of the polaron in the SQW are obtained by a method similar to that for the PQW.

Using Eqs. (11)–(14), we have numerically computed the energy levels of the ground and first excited states of a free polaron in a $GaN/Al_{0.3}Ga_{0.7}N$ PQWs and SQWs consisting of a wurtzite nitride material. The results are given in Figs. 1–3. The reference energy levels for the polaron are chosen at the bottom of the conduction band. In the numerical calculations, we use the value of GaN[22] as the parameters in the well material: $m_b/m_e = 0.19$, $\varepsilon_\perp^\infty = \varepsilon_z^\infty = 5.29$, $\omega_\perp = 69.56$ meV, $\omega_z = 66.08$ meV, $\omega_{\perp L} = 92.12$ meV, and $\omega_{zL} = 91.13$ meV. The parameters of the barrier material ($Al_{0.3}Ga_{0.7}N$) as obtained by the effective phonon-mode approximation[23] are $m_b/m_e = 0.238$, $\varepsilon_\perp^\infty = \varepsilon_z^\infty = 5.107$, $\omega_\perp = 73.72$ meV, $\omega_z = 70.81$ meV, $\omega_{\perp L} = 98.56$ meV, and $\omega_{zL} = 97.01$ meV.

We take account of the influence of the confined LO(TO)-like phonon modes and half-space LO(TO)-like phonon modes. The ground state energies as functions of the well width are shown in Fig. 1. The ground state energies decrease with increasing well width L rapidly at smaller L but slowly at larger L. The result for a wide well tends to the value for a 3D system. This behaviour is related to the change of the electron confinement in the quantum well. The ground energy level would be reduced by the effect of electron confinement with increase of well width. We also find that the phonons reduce the ground state energy of the electron. The effect of phonons is more important in wurtzite nitride semiconductors than that in AlGaAs. This result can also be obtained by analysing the contribution of different phonon modes to the ground state energy of the polaron. For comparison, we have also calculated the energy levels of the polaron in an infinite PQWs and the finite SQWs. The results are all plotted in Fig. 1. It can be seen that the energy levels in an infinite PQWs are larger than in a finite PQWs at smaller well widths, but the two are almost the same at large well widths. This characteristic is naturally similar to that in the SQWs. Moreover, the energy levels in the finite PQWs are higher than those in the finite SQWs. The results above are qualitatively similar to that of Ref. [17].

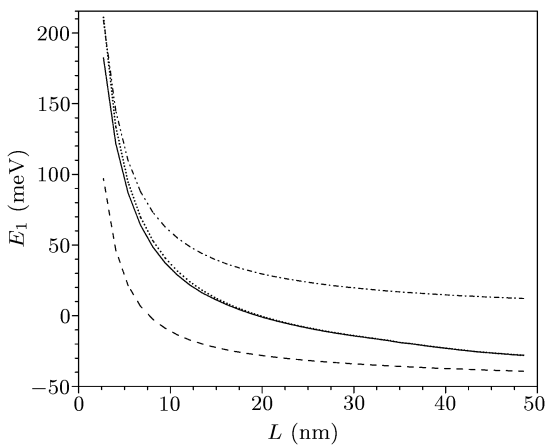


Fig. 1. Ground state energies of a polaron versus the well width L in a wurtzite $GaN/Al_{0.3}Ga_{0.7}N$ finite PQWs with (solid) and without (dot-dashed) phonon influence, in the infinite (dotted) PQWs and SQWs (dashed) with phonon influence.

Figure 2 shows the contributions of the LO (or TO)-like phonons, including the confined LO (or TO)-like phonon modes and the half-space LO (TO)-like phonon modes, to the energy of a polaron in the

wurtzite nitride finite PQWs. It can be found that the contribution from half-space LO-like phonon increases with decreasing well width, while the contribution from the confined LO-like phonons decreases. When the well becomes very narrow, the contribution from the half-space LO-like phonons rapidly increases and finally becomes much higher than that from the confined LO-like phonons. It can be easily understood that the confined electron tunnels strongly into the barrier and the overlapping between the wave function of the electron and the barrier phonons is broader for a narrower well, but the reversal is true for a wider well. This indicates that the contribution of confined LO-like phonons to the energy of the polaron is predominant in wider wells, and the contribution of half-space LO-like phonons becomes important in narrower wells. Meanwhile, we find that the total contributions of LO-like phonons reach a minimum in narrower wells. Also, the contribution from the TO-like phonon modes is not zero, but the contribution is smaller (about 0.2–0.4 meV) than that from the LO-like phonon modes (about 25–38 meV). Therefore, the contribution of the TO-like phonon modes to the energy of the polaron in the wurtzite nitride finite PQW structure is negligible.

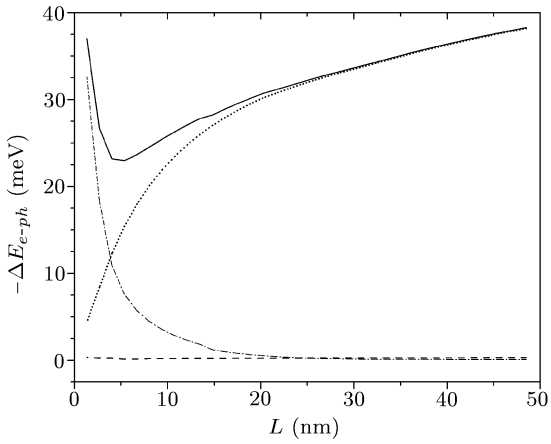


Fig. 2. Contributions of different kinds of phonons to the polaron energy-levels versus the well width L in the wurtzite $GaN/Al_{0.3}Ga_{0.7}N$ finite PQWs. The dot-dashed line is the curve of the half-space LO-like phonon contribution, the dotted line is the confined LO-like phonon contributions, the solid line is the total LO-like phonon contributions, and the dashed line is the total TO-like phonon contributions.

The first excited state energy and the transition energy of the polaron in the wurtzite nitride finite PQW structure as functions of the well width are plotted in Fig. 3. It can be seen that the first excited state energy and the transition energy decrease with increasing well width. The results of transition energy can be used to compare with experiment. An experimental observation for these properties in wurtzite PQW is invoked.

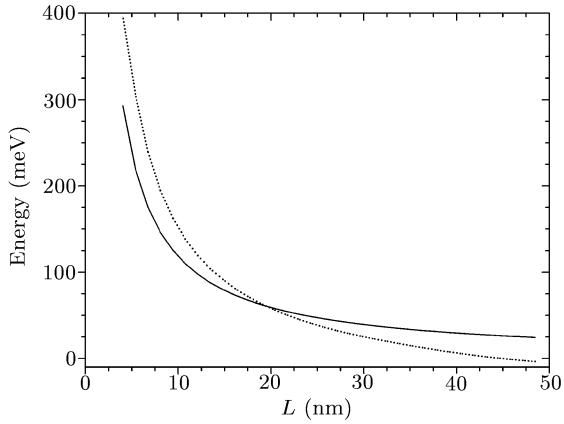


Fig. 3. The first excited state energies (dotted) and the transition energies (solid) of polarons with phonon influence versus the well width L in a wurtzite $GaN/Al_{0.3}Ga_{0.7}N$ finite PQW.

We have calculated the ground state energy, first excited state energy, and transition energy of a free polaron in a wurtzite $GaN/Al_{0.3}Ga_{0.7}N$ finite PQWs by taking account of the influence of confined LO(TO)-like phonon modes and half-space LO(TO)-like phonon modes, and considering the anisotropy of the all kinds of phonon modes. The contributions of all kinds of phonons to the energy of polaron are analysed in our calculation. It is found that the contribution of phonons to the energy of a polaron in wurtzite nitride PQWs is greater than that in an AlGaAs PQW. This indicates that the electron–phonon interaction in wurtzite nitride PQWs is not negligible.

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