# Effects of electron– and impurity-ion–LO phonon couples on the impurity states in cylindrical quantum wires*

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**Abstract:** The variational method and the effective mass approximation are used to calculate the phonon effects on the hydrogenic impurity states in a cylindrical quantum wire with finite deep potential by taking both the couplings of the electron-confined bulk longitudinal optical (LO) phonons and the impurity-ion–LO phonons into account. The binding energies and the phonon contributions are calculated as functions of the transverse dimension of the quantum wire. The results show that the polaronic effect induced by the electron–LO phonon coupling and the screening effect induced by the impurity-ion–LO phonon coupling tend to compensate each other and the total effects reduce the impurity binding energies.

**Key words:** quantum wire; electron-phonon interaction; impurity states
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## 1. Introduction

Recently, there has been an increasing interest in investigating quantum well wires (QWWs) both theoretically and experimentally due to the fact of their physical nature and their technological applications in electronics devices[1]. Many works are devoted to the study of the hydrogenic impurity states in both infinite[2–4] and finite deep potential[5–8] quantum wires with different geometries. It is found that the impurity binding energy in a quantum wire is much larger than that in a three-dimensional semiconductor. The phonon effects in low-dimension systems are important in determining the physical properties and have attracted much attention[9–19]. Buonocore *et al.*[9] and Xie[10] studied the polaron self-energies by considering both the volume and the surface phonon modes in cylindrical quantum wires with infinite potential. Moukhliss[11] chose infinitely deep potential wells to check the effect of the electron-confined bulk longitudinal optical (LO) phonon interaction on the ground bound state of the shallow donor impurity in a rectangular quantum wire. The impurity states in a quantum wire with a rectangular cross section and a finite barrier potential were also discussed by Osório *et al.*[12, 13]. The polar effects on the donor impurity binding energy in a cylindrical quantum wire with infinite[14] potential and finite[15] potential were analyzed by Xie *et al.* However, they missed the ion-phonon coupling when discussing the phonon effects. Recently, we[16] calculated the impurity ion–phonon coupling effect in a quantum wire, as pointed out by Platzman[17], and concluded that the screening of the impurity potential by the ion–phonon coupling reduces the binding energy and is much more important than the polaronic effect of the electron–phonon coupling. To the best of our knowledge, the phonon effect, taking both electron–phonon and ion–phonon coupling into account in a cylindrical quantum wire having a finite potential, has rarely been reported. Therefore, a detailed analysis is needed.

In this paper, we will study the binding energies of impurity states in polar cylindrical quantum wires with finite high potential by taking the LO phonon couplings with both, electrons and impurity ions, into account. The numerical results for the GaAs quantum wire will be shown and discussed.

## 2. Hamiltonian

Consider the GaAs QWW having a circular cross section of radius $R$ and the wire axis along the $z$-direction embedded in a dielectric matrix. An electron is bound to a hydrogenic donor impurity center in the wire. The Hamiltonian of the bound electron–LO phonon system can be expressed as

$$H = H_{\rm e} + H_{\rm LO} + H_{\rm e-LO}. \tag{1}$$

In Eq. (1), $H_{\rm e}$ is the Hamiltonian of the bare bound electron and can be written as

$$H_{\rm e} = -\frac{\hbar^2}{2m^*}\nabla^2 - \frac{e^2}{\varepsilon_\infty\sqrt{z^2+|\boldsymbol{r}-\boldsymbol{r}_{\rm i}|^2}} + V(r), \tag{2}$$

where $V(r)$ is the confining potential given by

$$V(r) = \begin{cases} 0, & r \leqslant R, \\ V_{\rm b}, & r > R. \end{cases} \tag{3}$$

In Eq. (2), the $\boldsymbol{r}$ direction is perpendicular to the axis of the wire, and $\boldsymbol{r}_{\rm i}$ gives the impurity's location along this direction. $\varepsilon_\infty$ is the high frequency dielectric constant and $m^*$ is the electron-band effective mass.

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$H_{\rm LO}$ in Eq. (1) is the Hamiltonian of the free phonon field of a confined LO phonon:

$$H_{\rm LO}=\sum_{mlk_z}\hbar\omega_{\rm LO}a^{\dagger}_{ml}(k_z)a_{ml}(k_z), \tag{4}$$

where $\omega_{\rm LO}$ is the LO phonon frequency, and $a^{\dagger}_{ml}$ and $a_{ml}$ are the corresponding creation and annihilation operators with the wave-vector $k_z$, respectively.

For the electron–LO interaction, we use the Hamiltonian derived by Wang and Lei[18] and take both the electron– and impurity ion–LO phonon couplings into account[17]. The last term in Eq. (1) can then be written as

$$H_{\rm e-LO}=\sum_{mlk_z}\left[\left(V^{*}_{\rm LO}(r)\,{\rm e}^{{\rm i}m\varphi}{\rm e}^{{\rm i}k_z z}-V^{*}_{\rm LO}(r_{\rm i})\right)a^{\dagger}_{ml}(k_z)+h.c.\right]. \tag{5}$$

Here, the impurity ion is assumed to be at rest and contributes the $-V^{*}_{\rm LO}(r_{\rm i})$ term to $H_{\rm e-LO}$. The coupling parameter in Eq. (5) is expressed as

$$V^{*}_{\rm LO}(r)=\Gamma^{*ml}_{\rm LO}(k_z)\,J_m\left(\frac{\chi^{l}_{m}}{R}r\right),\qquad r\leqslant R, \tag{6}$$

where

$$\Gamma^{*ml}_{\rm LO}=\frac{{\rm i}\sqrt{2}e\,(\hbar\omega_{LO})^{1/2}}{\sqrt{L}\sqrt{\chi^{l2}_{m}+k^{2}_{z}R^{2}}J_{m+1}\left(\chi^{l}_{m}\right)}\left(\frac{1}{\varepsilon_0}-\frac{1}{\varepsilon_\infty}\right)^{1/2}. \tag{7}$$

$J_m$ is the $m$-order Bessel function, and $\chi^{l}_{m}$ is the $l$-th root of $J_m$. $L$ is the length of the quantum wire. $\varepsilon_0$ is the static dielectric constant of the wire material.

We first treat the ion–phonon coupling term by performing the following canonical transformation, similarly to Ref. [17]:

$$U_0=\exp\left\{\sum_{mlk_z}(a^{\dagger}_{mlk_z}+a_{mlk_z})V^{*}_{\rm LO}(r_{\rm i})/\hbar\omega_{\rm LO}\right\}. \tag{8}$$

The transformed Hamiltonian is given by

$$\begin{aligned}H^{*}=&H_{\rm e}+\sum_{mlk_z}\hbar\omega_{\rm LO}a^{\dagger}_{mlk_z}a_{mlk_z}+\sum_{mlk_z}\left\{V^{*}_{\rm LO}(r){\rm e}^{{\rm i}k_z z}{\rm e}^{{\rm i}m\varphi}a^{\dagger}_{mlk_z}+h.c.\right\}\\&-\sum_{mlk_z}\left\{\frac{V_{\rm LO}(r)\,V_{\rm LO}(r_{\rm i})\,{\rm e}^{{\rm i}k_z z}{\rm e}^{{\rm i}m\varphi}}{\hbar\omega_{\rm LO}}+h.c.\right\}.\end{aligned} \tag{9}$$

Here, we have dropped the infinite constant self-energy term related to the positive point charge, $-\sum_{mlk_z}|V_{\rm LO}(r_{\rm i})|^2/\hbar\omega_{\rm LO}$, for convenience.

## 3. Binding energy of impurity states

To calculate the binding energy of impurity states, we perform Lee-Low-Pines(LLP)-like unitary transformations,

$$U_1=\exp\left[-{\rm i}\left(\sum_{mlk_z}k_z z a^{\dagger}_{mlk_z}a_{mlk_z}+\sum_{mlk_z}m\varphi a^{\dagger}_{mlk_z}a_{mlk_z}\right)\right], \tag{10}$$

and

$$U_2=\exp\left[\sum_{mlk_z}\left[f^{*}_{ml}(k_z)\,a_{ml}(k_z)-h.c.\right]\right], \tag{11}$$

where the variational parameters $f^{*}_{ml}$ and $f_{ml}$ can be determined by minimizing the expectation of the bound polaron Hamiltonian. The trial wave function is chosen as

$$|\Phi\rangle=\Psi(\boldsymbol{r})\,U_0U_1U_2\,|0\rangle, \tag{12}$$

where $|0\rangle$ is the phonon vacuum state, and $\Psi(\boldsymbol{r})$ the impurity state wave function chosen as

$$\Psi(\boldsymbol{r})=N\exp\left(-\lambda\sqrt{z^2+|\boldsymbol{r}-\boldsymbol{r}_{\rm i}|^2}\right)\begin{cases}J_0(\alpha r),\ r\leqslant R,\\ \dfrac{J_0(\alpha R)}{K_0(\beta R)}K_0(\beta r),\ r>R,\end{cases} \tag{13}$$

where $\lambda$ is the variational parameter, and $N$ the normalization constant of $\Psi(\boldsymbol{r})$. $\alpha$ and $\beta$ in Eq. (13) are determined by

$$\frac{\hbar^2\alpha^2}{2m^{*}}=V_{\rm b}-\frac{\hbar^2\beta^2}{2m^{*}}, \tag{14}$$

and the boundary condition on the wave function

$$\alpha\frac{{\rm d}J_0(\alpha r)}{{\rm d}(\alpha r)}\bigg|_{r=R}=\beta\,\frac{J_0(\alpha R){\rm d}K_0(\beta r)}{K_0(\beta R){\rm d}(\beta r)}\bigg|_{r=R}. \tag{15}$$

Minimizing $\langle\Phi|H|\Phi\rangle$ with respect to $f^{*}_{ml}(k_z)$, one can obtain

$$f_{ml}(k_z)=-\frac{\langle\Psi|\,\Gamma^{ml}_{LO}J_m\left(\dfrac{\chi^{l}_{m}}{R}r\right)|\Psi\rangle}{\hbar\omega_{\rm LO}+\dfrac{\hbar^2}{2m^{*}}\langle\Psi|\left(k^{2}_{z}+\dfrac{m^2}{r^2}\right)|\Psi\rangle-\dfrac{\hbar k_z P_z}{m^{*}}(1-\eta)}. \tag{16}$$

The variational energy of the ground state of the impurity states is then calculated by

$$\begin{aligned}\langle\Phi|\,H\,|\Phi\rangle=&\langle\Psi|\,\frac{P^{2}_{\rm r}}{2m^{*}}\,|\Psi\rangle+\langle\Psi|\,\frac{P^{2}_{z}}{2m^{**}}\,|\Psi\rangle+V(r)\\&-\langle\Psi|\,\frac{e^2}{\varepsilon_\infty\sqrt{z^2+|\boldsymbol{r}-\boldsymbol{r}_{\rm i}|^2}}\,|\Psi\rangle\\&-\sum_{mlk_z}\frac{\left|\langle\Psi|\,\Gamma^{ml}_{\rm LO}(k_z)\,J_m\left(\dfrac{\chi^{l}_{m}}{R}r\right)|\Psi\rangle\right|^2}{\hbar\omega_{\rm LO}+\dfrac{\hbar^2}{2m^{*}}\langle\Psi|\left(k^{2}_{z}+\dfrac{m^2}{r^2}\right)|\Psi\rangle}\\&-\sum_{mlk_z}\left\{\langle\Psi|\,\frac{V_{\rm LO}(r)\,V_{\rm LO}(r_{\rm i})\,{\rm e}^{{\rm i}k_z z}{\rm e}^{{\rm i}m\varphi}}{\hbar\omega_{\rm LO}}+h.c.\,|\Psi\rangle\right\},\end{aligned} \tag{17}$$

where $m^{**}$ is the renormalization mass of the electron in the direction along the wire:

$$m^{**}=\frac{m^{*}}{1-\eta}, \tag{18}$$

with

$$\eta=\frac{\Delta m_{LO}}{1+\Delta m_{LO}}, \tag{19}$$

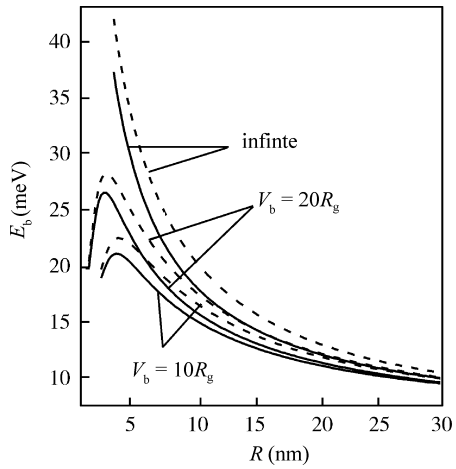


Fig. 1. Binding energies of the donor impurity states as a function of the wire radius with (solid lines) and without (dashed lines) the phonon contributions.

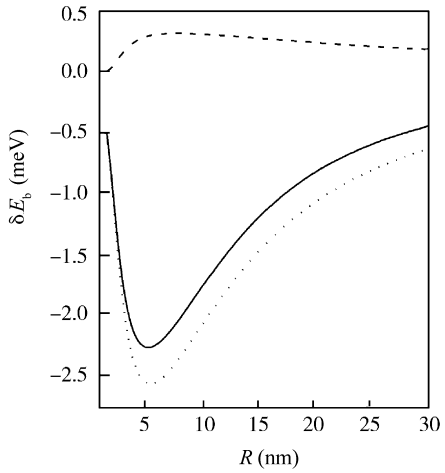


Fig. 2. Energy shifts of impurity states as a function of the wire, induced only by the electron–LO coupling (dashed line), only by the impurity-ion–LO coupling (dotted line), and both the electron– and ion–LO couples (solid line).

where $\Delta m_{\rm LO}$ is a dimensionless constant given by

$$\Delta m_{\rm LO} = \frac{2\hbar^2}{m^*} \sum_{mlk_z} \frac{k_z^2 \left| \langle \Psi | \, \Gamma_{\rm LO}^{ml}(k_z) \, J_m \left( \frac{\chi_m^l}{R} r \right) | \Psi \rangle \right|^2}{\left[ \hbar\omega_{\rm LO} + \frac{\hbar^2}{2m^*} \langle \Psi | \left( k_z^2 + \frac{m^2}{r^2} \right) | \Psi \rangle \right]^3}. \quad (20)$$

The ground state energy of the bound polaron can be calculated by

$$E_{\rm g} = \min_{\lambda} \langle \Phi | \, H \, | \Phi \rangle . \quad (21)$$

Denoting the free polaron energy in the quantum wire as $E_0$, the binding energy can be calculated as

$$E_{\rm b} = E_0 - E_{\rm g}. \quad (22)$$

The Hamiltonian of a free polaron in this system can be written as

$$\begin{aligned} H_{\rm free} &= H_{\rm e}^0 + H_{\rm LO}^0 + H_{\rm e-LO}^0 \\ &= -\frac{\hbar^2}{2m^*} \left( \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2} \right) - \frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2} + V(r) \\ &\quad + \sum_{mlk_z} \hbar\omega_{\rm LO} a_{ml}^{\dagger}(k_z) a_{ml}(k_z) \\ &\quad + \sum_{mlk_z} \left[ \Gamma_{\rm LO}^{ml}(k_z) \, J_m \left( \frac{\chi_m^l}{R} r \right) {\rm e}^{{\rm i}m\varphi} {\rm e}^{{\rm i}k_z z} a_{ml}^{\dagger}(k_z) + h.c. \right]. \end{aligned} \quad (23)$$

Using the LLP-like unitary transformation equations (10) and (11), the free polaronic energy can be variationally calculated as

$$\begin{aligned} E_0 &= \langle \Phi_0(r) | \, H_{\rm free} \, | \Phi_0(r) \rangle \\ &= \langle \Psi_0 | \, H_e^0 \, | \Psi_0 \rangle - \sum_{mlk_z} \frac{\left| \langle \Psi_0 | \, \Gamma_{\rm LO}^{ml}(k_z) \, J_m \left( \frac{\chi_m^l}{R} r \right) | \Psi_0 \rangle \right|^2}{\hbar\omega_{LO} + \frac{\hbar^2}{2m^*} \langle \Psi_0 | \left( k_z^2 + \frac{m^2}{r^2} \right) | \Psi_0 \rangle}, \end{aligned} \quad (24)$$

where $\Psi_0$ is the wave function of the bare electron in the cylindrical quantum wire:

$$\Psi(\boldsymbol{r}) = N_0 \begin{cases} J_0(\alpha r), & r \leqslant R, \\ \dfrac{J_0(\alpha R)}{K_0(\beta R)} K_0(\beta r), & r > R, \end{cases} \quad (25)$$

where $N_0$ is the normalization constant.

## 4. Numerical results and discussion

Calculations for the binding energies of impurity states are performed for the GaAs quantum wire. The parameters used in the calculations are $\varepsilon_0 = 13.18$, $\varepsilon_\infty = 10.89$, $m^* = 0.067m_0$ ($m_0$ is the free-electron mass), $\hbar\omega_{\rm LO} = 36.25$ meV, and $V_{\rm b} = 20R_{\rm g}$ ($R_{\rm g}$ is the effective Rydberg constant, $R_{\rm g} = m^* e^4 / 2\hbar^2 \varepsilon_0^2$).

We have plotted the binding energies of the impurity states in the GaAs quantum wires as a function of the wire radius with (solid lines) and without (dashed lines) phonon contributions for different barrier height potentials, $V_{\rm b} = 10R_{\rm g}$, $20R_{\rm g}$, and $\infty$, in Fig. 1. It is found that the binding energies of impurity states strongly depend on the size of the quantum wire. The binding energies increase starting at the values of the bulk GaAs material at large radii and reach a maximum at a radius, which is less than half the bound radius. It then decreases rapidly to the bulk values of the barrier material, when further decreasing the wire radius. One can clearly see that the binding energies in the infinite well are higher than those in a finite well. The effect of the barrier height is more significant for a smaller radius and less important in a wire with a bigger radius. When the barrier height is increased, the corresponding radius for the electron to leak to the barrier is becoming smaller. That is to say, when enhancing the barrier height, it is more difficult for an electron to leak to the barrier material; the probability to find the electron in the barrier material decreases. Consequently, the binding energy increases. For a

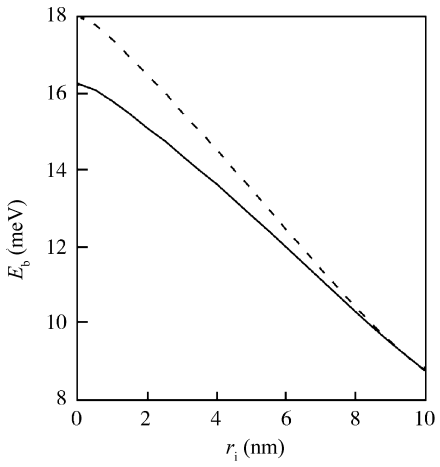


Fig. 3. Binding energies of impurity states as a function of the impurity position with (solid line) and without (dashed line) phonon contributions for $R$ = 10 nm.

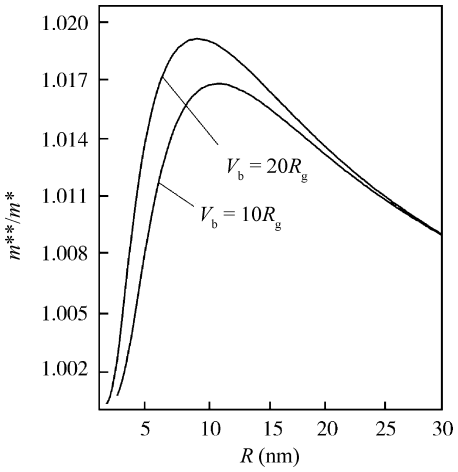


Fig. 4. Renormalization masses of the electron by LO phonons as functions of the wire radius in the GaAs quantum wire for $V_b = 10R_g$ and $20R_g$.

large quantum wire, all the curves will asymptotically approach the limit of the bulk value. One can also find that the binding energy with the phonon contributions (solid lines) is obviously lower than that without it (dashed lines).

To clearly see the influences of the electron– and ion–LO phonon couples on the binding energy of impurity states, we have plotted in Fig. 2 the shifts of the binding energies as functions of the wire radius, induced only by the electron–LO phonon coupling (dashed line), only the impurity-ion–LO phonon coupling (dotted line), and both the electron– and ion–LO phonon couples (solid line). One can see that the shifts of the binding energies with only the electron–LO phonon coupling (dashed line) and with only the impurity-ion–LO phonon coupling (dotted line) go into different directions. The former one is positive, and its absolute value is small; and the latter one is negative, and its absolute value is large. This means that the polaronic effect slightly enhances the impurity binding energy due to the increase in the effective mass of the electron induced by electron-phonon interaction. The energy shift induced by ion–LO phonon couples is significant (dotted line) because the ion–phonon interaction strongly screens the Coulomb potential and decreases the binding energy. When taking both the electron–phonon and the ion–phonon coupling into account (solid line), the binding energy is obviously changed. That is to say, the screening effect of the impurity center's potential is much stronger than the polaronic effect. The contrary effect of the two factors finally reduces the binding energy.

The binding energies of the impurity states as functions of the impurity position with (solid line) and without (dashed line) phonon contributions for $R$ = 10 nm are plotted in Fig. 3. The figure shows that the binding energies decrease rapidly when moving the impurity away from the center, which is due to the fact that the probability density of the electron around the impurity center is reduced. It is also seen that the phonon effect on the binding energy is larger when the impurity is located in the center and decreases as the impurity shifts away from the center because the phonon screening on the impurity's Coulomb potential is weakened.

In Fig. 4, we plot the renormalization masses of the electron by LO phonons as functions of the wire radius in the GaAs quantum wire for $V_b = 10R_g$ and $20R_g$. It is seen that the renormalization masses increase, reach a maximum, and then decrease rapidly, as the wire radius decrease. The phonon modification to the electron effective mass is still weak; though, it is larger when the barrier potential is higher (for $V_b = 20R_g$). Therefore, the correction of the binding energy induced by the renormalization mass is also weak.

## 5. Conclusion

In summary, we have investigated the impurity states in a cylindrical quantum wire with a finite high potential by taking both the electron–LO and ion–LO phonon coupling into account. The results show that the polaronic effect induced by the electron–LO phonon coupling and screen impurity potential effect induced by the impurity-ion–LO phonon coupling partially cancel each other. The shift of the binding energy induced by the ion–phonon coupling is significant. The polaronic effect is less important compared with the ion–LO phonon coupling.

## References

[1] Crouse D. Phonon modes and electron–phonon interactions in cylindrical quantum wires: macroscopic and microscopic analyses for device applications. J Appl Phys, 2006, 100(1): 014509

[2] Lee J, Spector H N. Hydrogenic impurity states in a quantum well wire. J Vac Sci Technol B, 1984, 2(1): 16

[3] Chuu D S, Hsiao C M, Mei W N . Hydrogenic impurity states in quantum dots and quantum wires. Phys Rev B, 1992, 46(7): 3898

[4] Bryant G W. Hydrogenic impurity states in quantum-well wires: shape effects. Phys Rev B, 1985, 31(12): 7812

[5] Bryant G W. Hydrogenic states in quantum-well wires. Phys Rev B, 1984, 29(12): 6632

[6] Brown J W, Spector H N. Hydrogen impurities in quantum wires. J Appl Phys, 1986, 59(4): 1179

[7] Kasapoglu E, Sari H, Sokmen I. Geometrical effects on shallow donor impurities in quantum wires. Physica E, 2003, 19(4): 332

[8] Chaudhuri S, Bajaj K K. Effect of nonparabolicity on the energy levels of hydrogenic donors in GaAs–$Ga_{1-x}Al_xAs$ quantum-well structures. Phys Rev B, 1984, 29(4): 1803

[9] Buonocore F, Iadonisi G, Ninno D, et al. Polarons in cylindrical quantum wires. Phys Rev B, 2002, 65(20): 205415

[10] Xie H J. Polaron self-energy and effective mass in a freestanding cylindrical quantum wire. Physica E, 2004, 22(4): 906

[11] Moukhliss S, Fliyou M, Sbai N E. Binding energy of the donor-confined LO phonon system in quantum well wire structures. Phys Status Solidi B, 1998, 206(2): 593

[12] Osório F A P, Degani M H, Hipólito O. Polaron effects on the impurity binding energy in quantum wires. Phys Rev B, 1995, 52(7): 4662

[13] Osório F A P, Degani M H, Hipólito O. Bound impurity in GaAs–$Ga_{1-x}Al_xAs$ quantum wires. Phys Rev B, 1988, 37(3): 1402

[14] Xie H J, Chen C Y, Ma B K. Bound polaron in a cylindrical quantum wire of polar crystal. Phys Rev B, 2000, 61(7): 4827

[15] Xie H J, Chen C Y, Ma B K. The bound polaron in a cylindrical quantum well with a finite confining potential. J Phys Condens Matter, 2000, 12(40): 8623

[16] Zhao Z R, Liang X X. On the ion– and electron–phonon interation effects on impurity states in polar cylindrical quantum wires. J Appl Phys, 2008, 103(5): 053704

[17] Platzman P M. Ground-state energy of bound polarons. Phys Rev, 1962, 125(6): 1961

[18] Wang X F, Lei X L. Polar-optic phonons and high-field electron transport in cylindrical GaAs/AlAs quantum wires. Phys Rev B, 1994, 49(7): 4780

[19] Klimin S N, Pokatilov E P, Fomin V M. Bulk and interface polarons in quantum wires and dots. Phys Status Solidi B, 1994, 184(2): 373