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LETTER TO THE EDITOR

The polaron self-energy and renormalized effective mass due to surface optical phonons in cylindrical quantum wires

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Abstract. We study electron–SO-phonon coupling in the case of Fröhlich interaction in cylindrical quantum wires. The polaron self-energy and renormalized effective mass due to surface optical phonons in cylindrical quantum wires have been calculated as functions of the radius of the wire by the standard LLP intermediate-coupling method. It is found that the strength of electron–SO-phonon coupling is strongly dependent on not only the size of the wires but also the dielectric constant of the surrounding medium. Our numerical results show that the effects of surface optical phonons are very significant and cannot be neglected in thin wires.

With the developments in microfabrication techniques, ultrasmall semiconductor quantum wires in which carriers are confined in two spatial directions have been successfully fabricated [1–3]. A great deal of interest has been shown in the study of these structures because of their potential device applications and their success in uncovering new phenomena.

The polaronic states are important in determining the physical properties of quantum wires, for example, in transport process or in inelastic electron scattering. The polaron effects of a Q1D electron gas interacting with confined bulk LO phonons in quantum wires have been studied. Ka-Di Zhu and Shi-Wei Gu [4] investigated the electron–LO-phonon interaction in quantum wires with rectangular cross section. Constantinou and Ridley [5] obtained the formula for the electron–LO-phonon interaction with circular cross section. They did not include the effects of the surface optical phonons, either. Hai *et al* [6] showed that the effects of the surface and interface phonons are significant and cannot be neglected in narrow quantum wells. So it may be predicted that the interaction of surface optical phonons and an electron cannot be neglected even in small quantum wires.

In th present paper, we investigate the polaronic states that incorporate the effects of surface optical phonons in GaAs quantum wires with circular cross section. Two different cases are investigated: (1) the wire is free-standing; (2) the wire is embedded in the surrounding medium.

First we give the Fröhlich interaction Hamiltonian for an electron interacting with surface optical phonons in a cylindrical quantum wire with radius ρ_0 and length L

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embedded in the surrounding medium of dielectric constant ϵ_d, which is derived by Zhou and Gu [7]

$$H_{e-so} = \sum_{m,k_z} \left[V_{e-SO}(\rho, m, k_z) \exp(im\phi) \exp(ik_z z) b_m(k_z) + \text{HC} \right] \tag{1}$$

where $b_m(k_z)$ is the annihilation operator for the m, k_z mode of surface optical phonons,

$$V_{e-SO}(\rho, m, k_z) = -\left[(1-\beta_e)/\omega_P\right]\left(e^2\hbar/L\omega_{SO}\right)^{1/2}\left(\omega_{SO}^2 - \omega_{TO}^2\right) \times I_m(\rho k_z)/\sqrt{\rho_0 k_z I_m(\rho_0 k_z) I'_m(\rho_0 k_z)} \tag{2}$$

and $\beta_e = \frac{4}{3} z\pi n\alpha_e$, $\omega_P^2 = 4\pi e^2 n/\mu$, α_e is the polarizability and ω_P is the ion plasma frequency.

The dispersion relation for the surface phonons is given by

$$\epsilon(\omega_{SO}) I'_m(\rho_0 k_z)/I_m(\rho_0 k_z) = \epsilon_d K'_m(\rho_0 k_z)/K_m(\rho_0 k_z) \tag{3}$$

where $I_m(x)$ and $K_m(x)$ are respectively the first-class and second-class Bessel functions with imaginary variables.

In many cases, the QID electron wave function is independent of ϕ, for example, within the spirit of the effective mass and parabolic-band approximation, the wave function is

$$\psi_e(\rho, z) = \left[\sqrt{2}/\rho_o J_1(x_0^{(1)})\right] J_0(x_0^{(1)}\rho/\rho_0) \exp(ik_z z)/\sqrt{2\pi} \tag{4}$$

where k_z is the wave number along the axis of the cylinder and $x_0^{(1)}$ is the first root of $J_0(x)$.

So, if we write $H_{e-SO} = \sum_m H^m_{e-SO}$, $\langle\psi_e|H^m_{e-SO}|\psi_e\rangle$ will be zero except for $m = 0$. We only need to take account of H^0_{e-SO}

$$H^0_{e-SO} = \sum_{k_z} \left[V_{e-SO}(\rho, k_z) \exp(ik_z z) b(k_z) + \text{HC} \right] \tag{5}$$

where we let $V_{e-SO}(\rho, k_z) = V_{e-SO}(\rho, k_z, m = 0)$.

The total Hamiltonian reads

$$H_P = H_e + H_{SO} + H_{e-SO}. \tag{6}$$

The first term is the Hamiltonian of the electron which is in the infinite well in the ρ direction and free in the z direction. It is given by

$$H_e = P_\rho^2/2m_b + V(\rho) + P_z^2/2m_b \tag{7}$$

where

$$V(\rho) = \begin{cases} \infty & \rho > \rho_0 \\ 0 & \rho < \rho_0 \end{cases}.$$

The second term is standard

$$H_{\mathrm{SO}} = \sum_{k_z} \hbar\omega_{\mathrm{SO}}(k_z) b^+(k_z) b(k_z). \tag{8}$$

Now, we introduce the following two unitary transformations:

$$U_1 = \mathrm{e}^{S_1} \qquad S_1 = -(\mathrm{i}/\hbar) z \sum_{k_z} \hbar k_z b^+(k_z) b(k_z) \tag{9}$$

$$U_2 = \mathrm{e}^{S_2} \qquad S_2 = \sum_{k_z} \left[g(k_z) b^+(k_z) - g^*(k_z) b(k_z) \right]. \tag{10}$$

Then the H_{P} can be transformed into

$$H_{\mathrm{P}} = U_2^{-1} U_1^{-1} H_{\mathrm{P}} U_1 U_2 = H_{\mathrm{e}} + \sum_{k_z} |g(k_z)|^2 \left[\hbar\omega_{\mathrm{SO}}(k_z) + \frac{\hbar^2 k_z^2}{2m_{\mathrm{b}}} - \frac{\hbar k_z}{m_{\mathrm{b}}} P_z \right] + \frac{1}{2m_{\mathrm{b}}} \left(\sum_{k_z} \hbar k_z |g(k_z)|^2 \right)^2 + H_{\mathrm{P}}' \tag{11}$$

where the part H_{P}' of the Hamiltonian H_{P} contains terms of no importance for the further calculations, and P_z is the projection of the total momentum of the polaron onto the z direction. It is easy to prove that P_z is a constant of the motion.

Defining the ground state of the electron–SO-phonon system in the low temperature limit

$$|\psi_{\mathrm{g}}\rangle = |\psi_{\mathrm{e}}\rangle |0\rangle \tag{12}$$

where $|\psi_{\mathrm{e}}\rangle$ is given in equation (4) and $|0\rangle$ is the vacuum state of SO phonons, we can get the ground energy of the polaron

$$E_{\mathrm{g}} = \langle \psi_{\mathrm{g}} | H_{\mathrm{P}} | \psi_{\mathrm{g}} \rangle. \tag{13}$$

Minimizing E_{g} by setting

$$\partial E_{\mathrm{g}} / \partial g(k_z) = \partial E_{\mathrm{g}} / \partial g^*(k_z) = 0 \tag{14}$$

we get

$$g(k_z) = -\langle\psi_e|V^*_{e\text{-SO}}(\rho, k_z)|\psi_e\rangle \Big/ \left[\hbar\omega_{SO}(k_z) + \hbar^2 k_z^2/2m_b - (\hbar k_z/m_b)P_z(1-\xi)\right] \tag{15}$$

$$\frac{\xi}{1-\xi} = \sum_{k_z} \frac{|\langle\psi_e|V_{e\text{-SO}}(\rho, k_z)|\psi_e\rangle|^2}{[\hbar\omega_{SO}(k_z) + \hbar^2 k_z^2/2m_b]^3} \frac{2\hbar^2 k_z^2}{m_b}. \tag{16}$$

Here, we introduce the coefficient γ which satisfies $\xi/(1-\xi) = \frac{1}{6}\alpha\gamma$. Finally

$$E_g = (\hbar^2/2m_b)\left(x_0^{(1)}/\rho_o\right)^2 + E_{tr} + P_z^2/2m_b^* \tag{17}$$

where E_{tr} is the polaron binding energy

$$E_{tr} = -\sum_{k_z} \frac{|\langle\psi_e|V_{e\text{-SO}}(\rho, k_z)|\psi_e\rangle|^2}{\hbar\omega_{SO}(k_z) + \hbar^2 k_z^2/2m_b} \tag{18}$$

and m_b^* is the polaron renormalized effective mass, $m_b^* = m_b(1 + \frac{1}{6}\alpha\gamma)$. Here we must point out that for bulk materials, m_b^* is equal to $m_b(1 + \frac{1}{6}\alpha)$ within the scope of intermediate coupling.

We now discuss the numerical results. We choose GaAs as an example to present the numerical results. In the calculations we have used the following parameters: a = 5.65 Å, $\hbar\omega_{LO}$ = 36.25 meV, $\hbar\omega_{TO}$ = 33.29 meV, ϵ_0 = 13.18, ϵ_∞ = 18.89, m_b/m_e = 0.067, α = 0.067 and the dielectric constant ϵ_d of the surrounding medium is 2.25.

Figure 1 shows the polaron self-energy as a function of the radius of the cylindrical quantum wire for two values of the dielectric constant ϵ_d of the surrounding medium. Two effects are pointed out here. Firstly, we can see from the figure that the absolute value of the polaron self-energy increases rapidly as the wire gets smaller. The reason for this is that the reduction of size leads to an increasing coupling to short-wavelength phonons. Comparing our results with those in [4], we find that for slim free-standing wires ($\rho_0 < 10a$), the absolute value of the polaron self-energy due to electron–LO-phonon interaction is less than that due to electron–SO-phonon interaction. Secondly, we find that the smaller the value of ϵ_d, the larger is the absolute value of the self-energy. This is because the dispersion relation $\omega_{SO}(k_z)$ for the SO phonon is strongly dependent on the value of ϵ_d.

Figure 2 shows the polaron renormalized effective mass as a function of the radius of the wire for two values of the dielectric constant ϵ_d. We find that it is similar to figure 1, but the polaron renormalized effective mass is more strongly dependent on the size of the wire than the self-energy is. As the wire becomes thicker, the coefficient γ decreases more rapidly. We also find that the value of the renormalized mass in thin wires is larger than that in a 3D system. So, we can see that for the same kind of material, the electron–phonon coupling in a Q1D system may be much stronger than that in a 3D system. As a result, for small wires, we must take into account the electron–SO-phonon interaction.

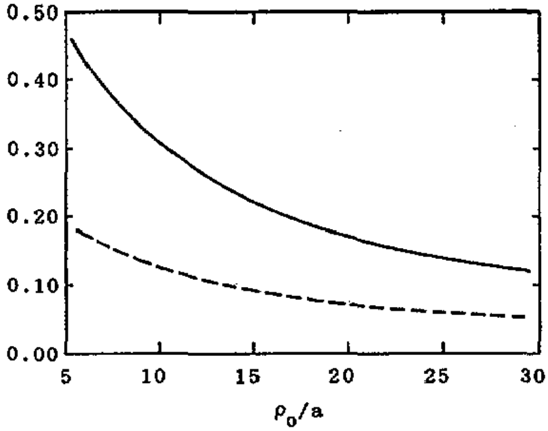

Figure 1. The polaron self-energy of GaAs quantum well wires with circular cross section in units of $-\alpha\hbar\omega_{SO}$ as a function of the radius of the wires: ——, E^1_{tr}, $\epsilon_d = 1.0$; - - - -, E^2_{tr}, $\epsilon_d = 2.25$.

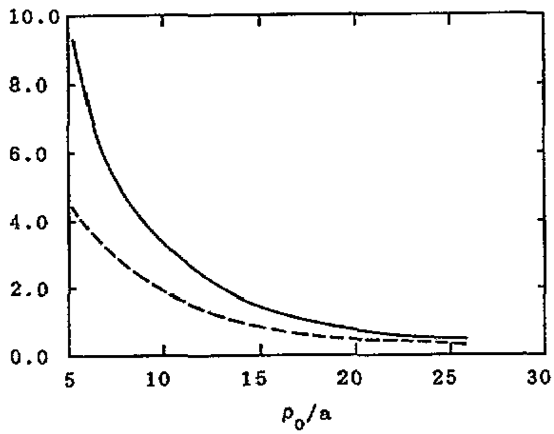

Figure 2. The polaron renormalized effective mass of GaAs quantum well wires with circular cross section as a function of the radius of the wires: ——, γ_1, $\epsilon_d = 1.0$; - - - -, γ_2, $\epsilon_d = 2.25$.

The polaron self-energy and its renormalized effective mass due to the interaction of an electron with the SO phonons in a cylindrical quantum-well wire have been calculated as functions of the radius of the wires by the LLP method. In the calculations, we have used the continuum approximation and effective mass approximation.

The results show that the effects of surface optical phonons are dominant in thin wires, and must be taken into account. We also find that the strength of electron–SO-phonon coupling is strongly dependent on the dielectric constant ϵ_d of the surrounding medium.

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