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Influence of Phonon Confinement on Line-width in Cylindrical Quantum Wires

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Abstract. Based on state-independent operator projection technique (SIOP) we calculate analytical expressions of conductivity tensor and absorption power in cylindrical quantum wires (CQW) due to the electron-longitudinal optical (LO) phonon interaction. Both electrons and phonons are confined in the CQW and numerical results are presented for free-standing GaAs/AlAs quantum wires. From graphs of the absorption power (AP) we obtain line-widths as profiles of curves. The dependence of the line-widths on the temperature and the radius of the CQW are obtained. Comparisons between the value of the absorption power and the line-widths in the case of confined phonons and bulk phonons are discussed.

Keywords: State-independent operator projection technique; cylindrical quantum wires; confined phonons; line-widths.

1. Introduction

Under the influence of high frequency electromagnetic field optical properties in quantum wires are defined by the interaction of electrons with optical phonons. Up to date, the number of works concerning the optical absorption in quantum wires in the case of confined phonon is still limited. This paper focuses on the influence of confined phonons on the line-width in cylindrical quantum wires. The absorption power (AP) is calculated by mean of the state-independent operator projection (SIOP) technique [1, 2]. The line-widths are defined by the profile of curves describing the dependence of absorption power on the photon energy. Since the expression of the form factor of electrons in the CQW is mathematically complicated when the phonon confinement is taken into account, in this paper we assume that electrons appear in the two lowest energy levels and the electron-electron interaction is neglected.

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2. Absorption power in cylindrical quantum wires with electron--bulk phonon interaction

In the action of the external field, $\vec{E}(t) = E_0 \exp\left[i(\omega t - kx)\right]\hat{z}$ which is polarized along z-direction, the optical conductivity tensor can be expressed by [1, 2]

$$\sigma_{zz}(\omega) = (i/\omega)\lim_{a\to 0^+} Tr\left\{\rho_{eq}\left[\left(\hbar\bar{\omega} - L\right)^{-1} J_z, J_z\right]\right\}, \tag{1}$$

where $\bar{\omega} \equiv \omega - ia$ $(a \to 0^+)$; Tr is the many body trace, $|\psi\rangle = (a_\alpha^+)^{n_\alpha}(a_\beta^+)^{n_\beta}...|\Phi_0\rangle$ is the state of a system including n_α particles in state $|\alpha\rangle$, n_β particles in state $|\beta\rangle$, and a_α^+ is the electron creation operator in this state; $|\Phi_0\rangle$ is the vacuum state; L is Liouville operator; ρ_{eq} is the equilibrium density operator. The many-electron current operator J_z can be written in term of the single-electron current operator j_z as $J_z = \sum_{\alpha,\beta} j_z^{\alpha\beta} a_\alpha^+ a_\beta$, where $j_z^{\alpha\beta} \equiv \langle\alpha|j_z|\beta\rangle$.

Using the expression of Hamiltonian of electron-bulk phonon system and SIOP technique, we can rewrite the conductivity tensor as [1]

$$\sigma_{zz}(\omega) = \frac{i}{\omega}\lim_{a\to 0^+} Tr\left|j_z^{\alpha\beta}\right|^2 \frac{f_\beta - f_\alpha}{\hbar\bar{\omega} - \left(E_\beta - E_\alpha\right) - \Gamma_{zz}(\bar{\omega})}, \tag{2}$$

where f_α is the electron distribution function of state $|\alpha\rangle$ with energy E_α.

It is noted that for CQW the electron energy spectrum is quantized in the plane perpendicular to the wire's axis, which is characterized by two quantum numbers ℓ and j. Function $\Gamma_{zz}(\bar{\omega})$ is called the line-shape function. Because this function is complex, we use Dirac identity to calculate the real part of the conductivity tensor

$$\mathrm{Re}\left[\sigma_{zz}(\omega)\right] = \frac{1}{\omega}\sum_{\alpha,\beta}\left|j_z^{\beta\alpha}\right|^2 \frac{\left(f_\alpha - f_\beta\right)B(\omega)}{\left[\hbar\omega - \left(E_\beta - E_\alpha\right)\right]^2 + \left[B(\omega)\right]^2}, \tag{3}$$

where $B(\omega)$ means the relaxation rate, which is defined by

$$\begin{aligned}
\left(f_\alpha - f_\beta\right)B(\omega) &= \pi\sum_q\sum_\gamma \left|C_{\beta\gamma}(q)\right|^2 \Big\{\left[\left(N_q+1\right)f_\alpha\left(1-f_\gamma\right) - N_q f_\gamma\left(1-f_\alpha\right)\right]\delta\left(\hbar\omega - E_\gamma + E_\alpha - \hbar\omega_q\right) \\
&+\left[N_q f_\alpha\left(1-f_\gamma\right) - \left(N_q+1\right)f_\gamma\left(1-f_\alpha\right)\right]\delta\left(\hbar\omega - E_\gamma + E_\alpha + \hbar\omega_q\right)\Big\} \\
&+\pi\sum_q\sum_\gamma \left|C_{\alpha\gamma}(q)\right|^2 \Big\{\left[\left(N_q+1\right)f_\gamma\left(1-f_\beta\right) - N_q f_\beta\left(1-f_\gamma\right)\right]\delta\left(\hbar\omega - E_\beta + E_\gamma - \hbar\omega_q\right) \\
&+\left[N_q f_\gamma\left(1-f_\beta\right) - \left(N_q+1\right)f_\beta\left(1-f_\gamma\right)\right]\delta\left(\hbar\omega - E_\beta + E_\gamma + \hbar\omega_q\right)\Big\} = B_1 + B_2 + B_3 + B_4
\end{aligned} \tag{4}$$

where N_q is the distribution of LO-phonons which are not confined; $C_{\beta\gamma}(q)$ is the electron-phonon interaction element matrix: $C_{\beta\gamma}(q) = C_q I_{\beta\gamma}(q) = 2\pi C_q I_{\ell_\beta j_\beta \ell_\gamma j_\gamma}(q_\perp)\delta_{k_{z\beta},k_{z\gamma}-q_z}$

For non-confined and dispersionless optical phonons, we have

$$\left|C_q\right|^2 = \frac{e^2\hbar\omega_{LO}}{2\chi_0 V}\left(\frac{1}{\chi_\infty} - \frac{1}{\chi_0}\right)\frac{1}{q_\perp^2 + q_z^2}, \tag{5}$$

where V is the volume of the specimen, χ_∞ and χ_0 are the dielectric constants corresponding to high and low frequency, respectively; ω_{LO} is the frequency of LO-phonon; $I_{\ell_\beta j_\beta \ell_\gamma j_\gamma}\left(q_\perp\right) = \left\langle \ell_\gamma, j_\gamma \left| e^{iq_\perp r_\perp} \right| \ell_\beta, j_\beta \right\rangle$ is the form factor of electrons between states β and γ.

Converting sums to integrals

$$\sum_\gamma \ldots \to \frac{L_z}{2\pi}\sum_{\ell_\gamma, j_\gamma}\int_{-\infty}^{+\infty} \mathrm{d}k_z \ldots, \qquad \sum_q \ldots \to \frac{V}{4\pi^2}\int_0^{+\infty} q_\perp \mathrm{d}q_\perp \int_{-\infty}^{+\infty} \mathrm{d}q_z \ldots, \tag{6}$$

we can calculate the first term in Eq. (4):

$$B_1 = \frac{L_z e^2 \hbar\omega_{LO} m^*}{4\hbar^2 \chi_0}\left(\frac{1}{\chi_\infty} - \frac{1}{\chi_0}\right)\sum_{\ell_\gamma, j_\gamma}\frac{1}{K_1}F_1\left\{Y_{11} + Y_{12}\right\}, \tag{7}$$

where

$$K_1 = \frac{1}{\hbar^2}\sqrt{2m^*\left(\hbar\omega - \hbar\omega_{LO} - E_{\ell_\gamma j_\gamma} + E_{\ell_\alpha j_\alpha}\right)}, \tag{8}$$

$$F_1 = \left(1 + N_q\right) f_\alpha \left\{1 - \left\{1 + \exp\left[\left(\hbar^2 K_1^2 / 2m^* + E_{\ell_\gamma j_\gamma} - E_F\right)/\left(k_B T\right)\right]\right\}^{-1}\right\}$$
$$- N_q\left(1 - f_\alpha\right)\left\{1 + \exp\left[\left(\hbar^2 K_1^2 / 2m^* + E_{\ell_\gamma j_\gamma} - E_F\right)/\left(k_B T\right)\right]\right\}^{-1}, \tag{9}$$

$$Y_{11} = \int_0^{+\infty}\left|I_{\ell_\beta j_\beta \ell_\gamma j_\gamma}\left(q_\perp\right)\right|^2 \frac{1}{q_\perp^2 + \left(K_1 - k_{z\beta}\right)^2} q_\perp \mathrm{d}q_\perp, \tag{10}$$

$$Y_{12} = \int_0^{+\infty}\left|I_{\ell_\beta j_\beta \ell_\gamma j_\gamma}\left(q_\perp\right)\right|^2 \frac{1}{q_\perp^2 + \left(K_1 + k_{z\beta}\right)^2} q_\perp \mathrm{d}q_\perp. \tag{11}$$

In Eq. 5 the quantities e, m^* and E_F are respectively the charge, mass of electron, Fermi energy, k_B being the Boltzmann constant and T - the temperature of the system. The terms B_2, B_3, B_4 in (4) are calculated in the similar way.

We finally obtain the expression of $\mathrm{Re}\left[\sigma_{zz}\left(\omega\right)\right]$ in CQW by using approximate calculation of integrals. The AP is calculated in the same way as [3]

$$P = \frac{E_0^2}{2}\mathrm{Re}\left[\sigma_{zz}\left(\omega\right)\right]. \tag{12}$$

In a CQW with radius *R*, we consider two lowest levels in which $x = Rq_{\perp}$ and $Q_1 = R\left(K_1 - k_{z\beta}\right)$ and obtain

$$Y_{11} = \int_0^{+\infty} \left|I_{\pm1,1,0,1}\left(x\right)\right|^2 \frac{1}{x^2 + Q_1^2} x\mathrm{d}x = 48^2 \int_0^{+\infty} \frac{J_4^2\left(x\right)}{x^5\left(x^2 + Q_1^2\right)}\mathrm{d}x. \tag{13}$$

This kind of integral has been already calculated in Ref. 4

$$Y_{11} = \frac{48^2}{Q_1^6}\left[\frac{1}{8} - \frac{Q_1^2}{240} + \frac{Q_1^4}{3840} - I_4\left(Q_1\right)K_4\left(Q_1\right)\right], \tag{14}$$

where $I_4\left(Q_1\right)$ and $K_4\left(Q_1\right)$ are modified Bessel functions. If we determined the expression of $Y_{\gamma\delta}$ ($\gamma = 1,2,3,4$; $\delta = 1,2$) we shall obtain the one for $B\left(\omega\right)$, and then the one for AP in the case of bulk phonons in Eq. (10).

3. Absorption power in the case of electron-confined phonon interaction

The calculating method for this case is the same as that for the bulk phonon case. The phonon wave vector is now quantized, $q_{\perp} = q_{m,n}$. The expression of $Y_{\gamma\delta}$ in the case of $\delta = 1$ becomes

$$Y_{\gamma1} = \sum_{q_{m,n}} \frac{\left|I^C_{\ell,j,\ell',j'}\right|^2 q_{m,n}}{\left(K_\gamma - q_z\right)^2 + q_{m,n}^2}, \qquad Y_{\gamma2} = \sum_{q_{m,n}} \frac{\left|I^C_{\ell,j,\ell',j'}\right|^2 q_{m,n}}{\left(K_\gamma + q_z\right)^2 + q_{m,n}^2}, \tag{15}$$

where $I^C_{\ell,j,\ell',j'}\left(\eta\right) = \frac{2}{J_{\left|\ell-\ell'+1\right|}\left(A_{\ell-\ell',n}\right)} \int_0^1 \varepsilon \mathrm{d}\varepsilon \frac{1}{y_{\ell j} y_{\ell' j'}} J_\ell\left(A_{\ell j}\varepsilon\right) J_{\ell-\ell'}\left(\eta\varepsilon\right) J_{\ell'}\left(A_{\ell' j'}\varepsilon\right)$,

with $A_{\ell j}$ is the j^{th} real root of Bessel *J* function of order ℓ, $\eta = q_{m,n}R$, $\varepsilon = r/R$, $y_{\ell j} = J_{\ell+1}\left(A_{\ell j}\right)$ and $y_{\ell' j'} = J_{\ell'+1}\left(A_{\ell' j'}\right)$.

Because $x = Rq_{m,n}$ and $q_{1,n} = A_{1n}/R$, $x \equiv A_{1n}$ then $Q_{\gamma1} = R\left(K_\gamma - q_z\right)$ is quantized [5]. Suppose that electrons occupy the lowest levels, we have $I^C_{\pm1,1,0,1} = 48 J_4\left(q_{m,n}R\right) / \left(J_2\left(A_{1n}\right)\left(q_{m,m}R\right)^3\right)$. The expression of $Y_{\gamma1}$ now becomes:

$$Y_{\gamma1} = 48^2 \sum_n \frac{J_4^2\left(A_{1n}\right)}{J_2^2\left(A_{1n}\right)} \frac{1}{x^5\left(x^2 + Q_{\gamma1}^2\right)}. \tag{16}$$

Converting the sum into the integral, we obtain

$$Y_{\gamma 1} = 48^2 \left\{ \sum_{n=1}^{5} \frac{J_4^2(A_{1n})}{J_2^2(A_{1n})} \frac{1}{(A_{1n})^5 \left[(A_{1n})^2 + Q_{\gamma 1}^2 \right]} + \frac{1}{\pi} \int_{19}^{+\infty} \frac{1}{x^5 \left(x^2 + Q_{\gamma 1}^2 \right)} \mathrm{d}x \right\}. \tag{17}$$

The expression of $Y_{\gamma 2}$ are defined by the similar method. From these we can obtain $B(\omega)$ and AP expression in the case of confined LO phonons.

4. Numerical results and discussion

For numerical computation we used [5,6]: $m^* = 6.097 \times 10^{-32}$ kg, $\chi_\infty = 10.9$, $\chi_0 = 13.1$, $\hbar\omega_{LO} = 36.25$ meV, $L_z = 100$ nm, $E_0 = 10^5$ V/m, $E_F = 0.5 \times 10^{-18}$ J.

Figure 1 shows the dependence of AP in GaAs/AlAs CQW on photon energy in the case of bulk phonons and confined phonons. We can see from the figure that the energy dependence of AP has resonant peak which is similar to the graph of Gauss or Lorentz function. This is the reason why we can obtain the line-widths by curve profiles. It can be seen from the figure that the AP increases with temperature (the resonant peak is lifted), while the resonant peak positions remain constant at the energy value of $\hbar\omega_{LO} = 19.80$ meV. From the expression of electron energy in cylindrical quantum wire $E_{n,\ell} = \hbar^2 A_{n\ell}^2 / (2m^* R^2)$, we can obtain $\Delta E_{\beta\alpha} = E_\beta - E_\alpha = 19.80$ meV for *R*=16nm. Consequently, these resonant peaks satisfy the condition $\hbar\omega = \Delta E_{\beta\alpha}$.

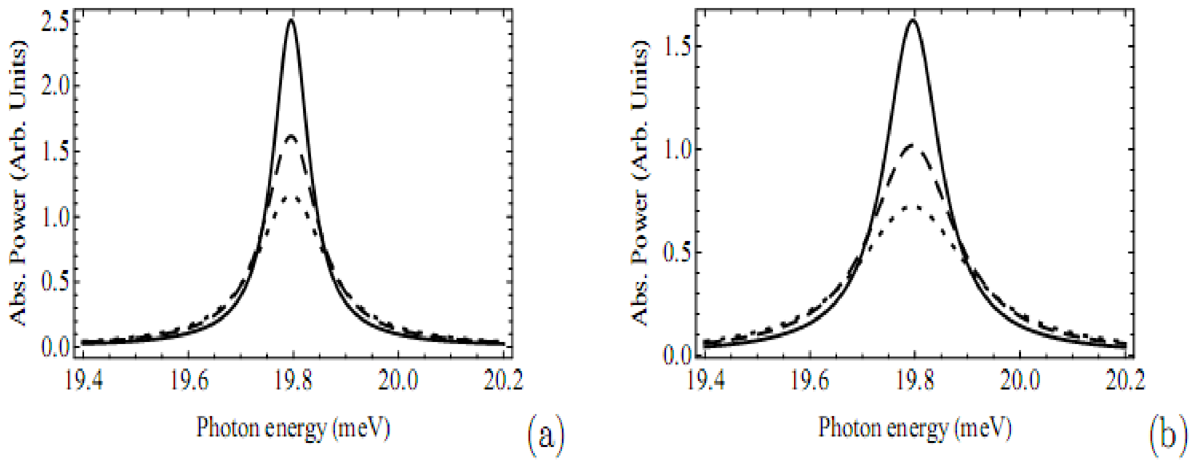

Figure 1. Absorption power in GaAs/AlAs CQW of R=16 nm with three values of temperature:the solid, dotted, and dashed lines correspond to 200 K, 250 K, and 300 K, respectively, for bulk phonons (a) and confined phonons (b)

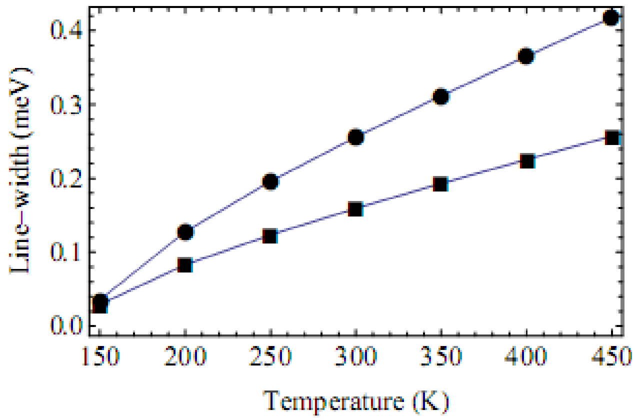

Figure 2. Comparison of the line-widths in GaAs/AlAs CQW with R =16 nm in the case of bulk phonons (the square line) and con¯ ned phonons (the circle line).

Using the method presented in our previous paper [7], we obtain the temperature dependence of line-widths as shown in Fig. 2. From this figure we can see that when temperature increases, the electron-LO phonon scattering probability increases. This result is the same as that obtained in the two dimensional system which is verified by theories and experiments [3,8]. Beside, Fig. 2 shows that the value of line-width in the case of confined phonons is greater that in the case of bulk phonons. This can be explained by the fact that the electron-confined phonon scattering probability increases, as the result, the line-widths become greater.

Figure 3(a) shows the dependence of the AP on photon energy with different values of wire's radius in the case of confined phonons. We can see from the figure that as R increases the peak shifts to the lower energy. With R = 14 nm, 16 nm, and 18 nm the photon energy values corresponding to resonance peaks are $\hbar\omega$=25.86meV, 19.80meV, and 15.64meV. As R increases, $\Delta E_{\beta\alpha}$ decreases. Consequently, the photon energy satisfying the resonance condition $\hbar\omega = \Delta E_{\beta\alpha}$ decreases.

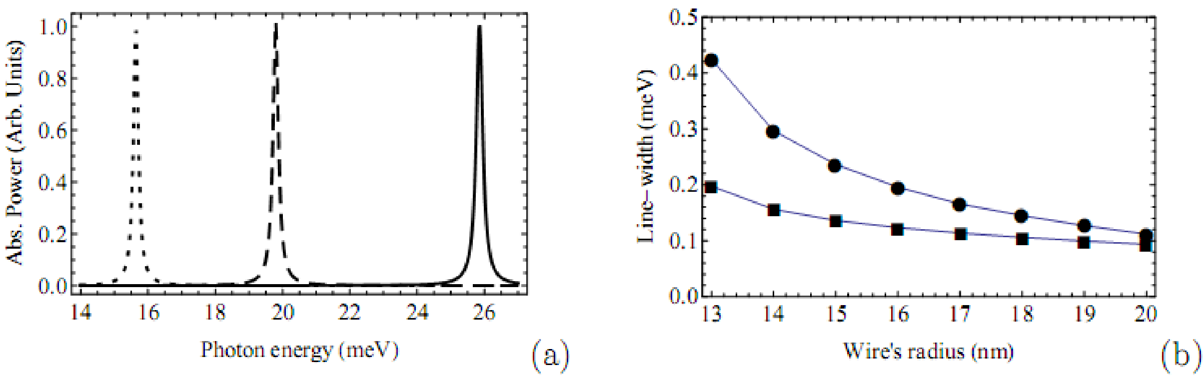

Figure 3. (a) Absorption power in GaAs/AlAs CQW at T =250K: the solid, dotted, and dashed lines correspond to radius R =14 nm, 16 nm, and 18 nm for the case of con¯ ned phonons. (b) Comparison of the line-widths in GaAs/AlAs CQW with T = 250 K in the case of bulk phonons (the square line) and confined phonons (the circle line).

Figure 3(b) shows the dependence of the line-widths on the wire's radius. It can be seen from the figure that the line-widths decrease as the wire's radius increases. This can be explained by that fact that as the wire's radius increases, the confinement of electrons is looser, therefore the electronic mobility is increased and so are the line-widths. In addition, Fig. 3(b) also shows that the value of line-width in the case of confined phonons is greater and asymptotic to that in the case of bulk phonons when R increases. The reason for this is that when phonons are confined, the electron-phonon scattering probability increases significantly, so that the line-widths increase. Moreover, when the wire's radius increases the electron-phonon interaction decreases sharply and the confinement of phonons disappears.

5. Conclusion

In the present paper, we calculated analytical expressions of conductivity tensor and absorption power in CQW due to electron-LO phonon interaction in both case bulk and confined phonons.

From the graphs of the absorption power $P(\omega)$, we obtained the line-widths as profiles of curves. Computational results show that, in both case of bulk and confined phonons the line-widths increase with temperature and decrease with wire's size. In addition, the value of line-widths in the case of confined phonons is greater and asymptotic to that in the case of bulk phonons when R increases. This result is the same as that obtained in the two dimensional system which is verified by theories and experimentations.

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