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Optical phonon modes in a free-standing quantum wire with ring geometry

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ABSTRACT

The confined longitudinal-optical (LO) phonon and surface-optical (SO) phonon modes of a free-standing quantum wire with ring geometry are discussed within the dielectric continuum (DC) approximation. Two branches of SO phonon modes have been investigated. The frequencies of the SO phonons are found to be dispersed and radius dependent for small size systems. When the wave vector $q_z \to \infty$, the frequencies of each SO modes converge to the frequency values of the single planar heterostructure.

1. Introduction

With the rapid progress in semiconductor nanotechnology, such as with molecular-beam epitaxy, metal-organic chemical-vapour deposition and chemical lithography, various kinds of low-dimensional microstructure including quantum wells (QWs), quantum well wires (QWWs) and quantum dots (QDs) can be fabricated. Due to their potential technological application, much attention have been attached to these low-dimensional structure [1–6]. In these low-dimensional quantum systems, it is well known that the phonons are also confined, which makes the phonon modes more complicated than those in the bulk materials [7]. Furthermore, the electron–phonon interaction in these confined systems is one of the important aspects in determining their properties in physical processes, such as in the transport process or the electron relaxation process. Therefore, in order to describe the coupling between electron and phonon properly in these low-dimensional quantum systems, a well-known phonon mode and electron–phonon interaction Hamiltonian are essential.

Since the pioneering work of Licari [8] and Fuchs [9] on the phonon modes in confined quantum systems, several authors have made their contributions to studying the phonon modes and electron–phonon interaction. Various theoretical models, such as the dielectric continuum (DC) model [8,10–12], hydrodynamic model [13], and microscopic calculation modes [14] have been adopted. The DC model had been widely used for its simplicity and efficiency. Mori and Ando [15] have investigated the phonon modes in single- and double-heterostructure QWs within the framework of the DC approach. Liang and Wang [16] have derived the transverse-optical (TO) and longitudinal-optical (LO) modes as well as four branches of interface optical modes in a GaSb–InAs–GaSb QW. Klein [17] and Roca [18] have derived the polar optical phonon modes for spherical quantum dots. Cruz [19,20] has obtained the interface-optical (IO) phonon in GaAs/$Al_xGa_{1-x}As$ quantum spheres and derived the surface optical (SO) phonon modes in free standing rectangular quantum boxes. Zhou et al. [21] have derived the IO phonon modes in a rectangular QD's embedding in other polar material. Xie and Chen [22] have derived the IO and SO phonon mode in a quantum well wires. Li and Chen [23] have derived the LO, TSO (top surface optical) and SSO (side surface optical) modes in a freestanding cylindrical quantum dots. Zhang et al. [24] have derived the LO and IO (SO) phonon modes in a multi-shell sphere quantum dots.

In the present Letter, we derived the general expressions of the phonon modes, the dispersion relation, and electron–phonon Fröhlich interaction Hamiltonian in a free-standing quantum wire with ring geometry within the framework of dielectric continuum approximation. Result reveals that there exist two branches of SO modes which are localized at the inner and outer radius respectively. The frequencies of the SO phonons are found to be dispersed with small wave-vector q_z. With increasing q_z, the frequency of each SO modes approaches the frequency values of single planar

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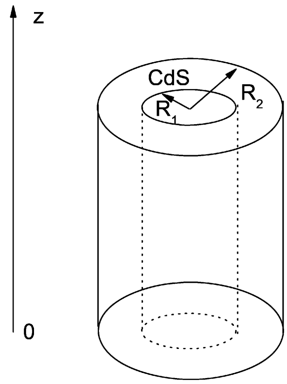

Fig. 1. The shape of a free-standing cylindrical quantum wire with a ring geometry.

heterostructure. Especially, other than the quantum wire systems studied by Xie and Chen [22] in which the frequencies of the SO phonons are radius independent, in our system the frequencies for both of the SO modes are size dependent for the small well-width. This Letter is organized as follows: In Section 2, the Fröhlich electron–SO (LO) phonon interaction Hamiltonian and the SO phonon dispersion relations were derived. In Section 3, the numerical calculations were performed on the CdS quantum wire, and the dependence of the dispersion frequencies and the coupling intension for the SO phonon modes on the wave-vector q_z, the quantum number m and the size of the system were given and discussed. Finally, in the last section, a brief summary is given.

2. Model and theory

As shown in Fig. 1 we consider a free-standing cylindrical quantum wire with ring geometry. The inner and outer radius are R_1 and R_2, respectively; the length of the wire is L, which satisfied $L \gg R_2$. Under the continuum approximation, we will derive an expression for Fröhlich interaction in our system of concern. We start with the electrostatic equations

$$\nabla \cdot \boldsymbol{D} = 4\pi\rho_0(\boldsymbol{r}), \tag{1}$$

$$\boldsymbol{D} = \epsilon\boldsymbol{E} = \boldsymbol{E} + 4\pi(\boldsymbol{P}), \tag{2}$$

$$\boldsymbol{E} = -\nabla\phi, \tag{3}$$

where $\boldsymbol{D}$, $\boldsymbol{E}$, $\boldsymbol{P}$ and ϕ are the electric displacement, electric field, electric polarization density and electric potential, respectively. ρ_0 is the charge density and ϵ is the dielectric constant of the annulus wires. From the above equations, we can get

$$\epsilon\nabla^2\phi(\boldsymbol{r}) = 0, \tag{4}$$

for free oscillation.

2.1. The LO vibrational eigenmodes

There are two possible solutions for Eq. (4), one of which is $\epsilon = 0$ inside the wire. Since in a polar crystal,

$$\epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_0 - \epsilon_\infty}{1 - \frac{\omega^2}{\omega_{\mathrm{TO}}^2}}, \tag{5}$$

where ϵ_0 and ϵ_∞ are the static and high-frequency dielectric constants and ω_{TO} is the frequency of the TO phonon, $\epsilon = 0$ would give

$$\omega^2 = \omega_{\mathrm{TO}}^2\frac{\epsilon_0}{\epsilon_\infty} = \omega_{\mathrm{LO}}^2. \tag{6}$$

Eq. (6) is just the Lyddane–Sachs–Teller (LST) relation, which describes the bulk LO modes of frequency $\omega = \omega_{\mathrm{LO}}$. In this case, the electric potential in Eq. (4) is an arbitrary function of $\boldsymbol{r}$. The eigenfunctions of the confined LO phonon can be chosen as

$$\phi_{ml}(\boldsymbol{r}) = \begin{cases} A_{ml}\tau_{ml}(\frac{a_{ml}\rho}{R_1})e^{-im\varphi}e^{-iq_z z}, & R_1 \leqslant \rho \leqslant R_2, \\ 0, & \text{otherwise}, \end{cases}$$
$$\tau_{ml}\left(\frac{a_{ml}\rho}{R_1}\right) = J_m\left(\frac{a_{ml}\rho}{R_1}\right) + b_{ml}N_m\left(\frac{a_{ml}\rho}{R_1}\right), \tag{7}$$

where $J_m(x)$ and $N_m(x)$ are the mth-order Bessel and Neumann functions; A_{ml}, a_{ml} and b_{ml} can be determined by the boundary conditions of electrostatic at $\rho = R_1, R_2$.

The polarization vectors ($\boldsymbol{P} = \nabla\phi/4\pi$) for confined LO mode are calculated by considering Eqs. (2) and (3) and the condition $\epsilon = 0$. We get

$$\begin{aligned} \boldsymbol{P}_{ml}^{\mathrm{LO}} &= \frac{1-\epsilon}{4\pi}\nabla\phi_{ml}(\boldsymbol{r}) \\ &= \frac{1-\epsilon}{4\pi}A_{ml}\left\{\frac{1}{2}\left[\tau_{m-1,l}\left(\frac{a_{ml}\rho}{R_1}\right) - \tau_{m+1,l}\left(\frac{a_{ml}\rho}{R_1}\right)\right]\frac{a_{ml}\rho}{R_1}\boldsymbol{e}_\rho \right. \\ &\quad \left. - \frac{im}{\rho}\tau_{ml}\left(\frac{a_{ml}\rho}{R_1}\right)\boldsymbol{e}_\varphi - iq_z\tau_{ml}\left(\frac{a_{ml}\rho}{R_1}\right)\boldsymbol{e}_z\right\}e^{-im\varphi}e^{-iq_z z}. \end{aligned} \tag{8}$$

To derive the free phonon Hamiltonian, we need the dynamic equations of motion of the crystal lattice [15,17,25]:

$$\mu\ddot{\boldsymbol{u}} = -\mu\omega_0^2\boldsymbol{u} + e\boldsymbol{E}_{\mathrm{loc}}, \tag{9}$$

$$\boldsymbol{P} = n^*e\boldsymbol{u} + n^*\alpha\boldsymbol{E}_{\mathrm{loc}}, \tag{10}$$

where μ is the reduced mass of the ion pair and $\boldsymbol{u} = \boldsymbol{u}_+ - \boldsymbol{u}_-$ is the relative displacement of the positive and negative ions, ω_0 is the frequency associated with the short-range force between ions, n^* is the number of ion pairs per unit volume, and α is the electronic polarizability per ion pair, $\boldsymbol{E}_{\mathrm{loc}}$ is the local field at the position of the ions.

The Hamiltonian of the free vibration is given by

$$H_{\mathrm{ph}} = \frac{1}{2}\int d^3r\left(n^*\mu\dot{\boldsymbol{u}}\cdot\dot{\boldsymbol{u}} + n^*\mu\omega_0^2\boldsymbol{u}\cdot\boldsymbol{u} - n^*e\boldsymbol{u}\cdot\boldsymbol{E}_{\mathrm{loc}}\right). \tag{11}$$

We have made use of the harmonic approximation for $\boldsymbol{P}$, $\boldsymbol{u}$, and $\boldsymbol{E}_{\mathrm{loc}}$.

The local field in macroscopic approach is [25]

$$\boldsymbol{E}_{\mathrm{loc}} = -\frac{8}{3}\pi\boldsymbol{P}. \tag{12}$$

$\boldsymbol{E}_{\mathrm{loc}}$ is the electric field associates with the LO vibrational mode. Combining Eqs. (10) and (12), we have

$$\boldsymbol{u} = \frac{1 + (8/3)\pi n^*\alpha}{n^*e}\boldsymbol{P}. \tag{13}$$

Hence, the confined LO phonon Hamiltonian from Eq. (11) can be written as

$$\begin{aligned} H_{\mathrm{LO}} = \frac{1}{2}\int d^3r\Bigg[&n^*\mu\left(\frac{1 + (8/3)\pi n^*\alpha}{n^*e}\right)^2\dot{\boldsymbol{P}}^*\cdot\dot{\boldsymbol{P}} \\ &+ n^*\mu\omega_{\mathrm{LO}}^2\left(\frac{1 + (8/3)\pi n^*\alpha}{n^*e}\right)^2\dot{\boldsymbol{P}}^*\cdot\dot{\boldsymbol{P}}\Bigg]. \end{aligned} \tag{14}$$

The LO polarization vectors from Eq. (8) form an orthonormal and complete set:

$$\begin{aligned} &\int d^3r\,2n^*\mu\left(\frac{1 + (8/3)\pi n^*\alpha}{n^*e}\right)^2\boldsymbol{P}_i^{mlq_z*}\cdot\boldsymbol{P}_j^{m'l'q_z'} \\ &\quad = \delta_{ij}\delta_{mm'}\delta_{ll'}\delta_{q_zq_z'}, \end{aligned} \tag{15}$$

from which A_{ml} can be determined,