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Electron–interface-optical-phonon interaction in rectangular quantum wire and quantum dot

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ABSTRACT

Under the dielectric continuum model and separation of variables, the interface optical (IO) phonon modes and electron–optical-phonon interaction in rectangular quantum wire and quantum dot embedded in a nonpolar matrix are studied. We found that there exist various types of IO phonon modes in rectangular nanostructures. The IO phonon modes in rectangular quantum wire include IO–propagating (IO–PR) and IO–IO hybrid phonon modes, while the IO phonon modes in rectangular quantum dot contain IO–IO–PR and IO–PR–PR hybrid phonon modes. The results of numerical calculation show that these hybrid phonon modes contain corner optical (CO) phonon modes and edge optical (EO) phonon modes. The potential applications of these results are also discussed.

1. Introduction

Currently, many fabricating technologies such as metal-organic chemical vapor deposition, molecular beam epitaxy, and vapor–liquid–solid growth have been developed for fabricating nanostructures with a wide range of sizes, shapes, and dielectric environments. The nanobelts [1], triangular nanowires [2], tetrapod nanocrystals [3], nanocombs [4], nanorings [5], nanobridges and nanonails [6] have been synthesized. It is of great interest to research the effect of shape on their physical properties, because nanomaterials of complex shapes have different crystallographic facets and different fraction of surface atoms on their corners and edges, which contributes significantly to modulating their physical properties. On the other hand, the optical phonon modes and electron–phonon interaction play a key role in many physical properties of the polar crystals such as the binding energy of impurities, carrier transportation, linear and nonlinear optical properties, especially in low-dimensional materials. So, it is of practical interest to research polar optical phonon modes and the electron–optical-phonon interaction Hamiltonian for quantum systems of complex shapes.

There exist different kinds of phonon modes in nanomaterials with different crystallographic facets and shapes, e.g., confined longitudinal optical (LO) modes, surface optical (SO) and interface optical (IO) modes. Particularly, for nanostructures with edges and corners, the so-called edge optical (EO) modes [7] and corner optical (CO) modes [8,9] have been found. By studying quantum wires with the dielectric continuum (DC) model [10–14], Knipp and Reinecke [9] have found that the CO phonon modes localize in the corners of the wires or regions of high curvature, and the degree of localization increases with the increasing sharpness of the corners. So, the EO or CO phonon modes should exist in quantum systems of complex shapes including corners. Both the isotropic materials of different shapes [15–23] and the wurtzite-type anisotropic materials [24–34] have been studied extensively with the DC model, because the DC model provides analytic expressions for the phonon eigenfunctions, phonon frequencies, and Fröhlich Hamiltonian between the electron and phonon conveniently. On the other hand, the rectangular quantum wire and quantum dot which have edges and corners are candidates for studying optical phonon modes in quantum systems of complex shapes. Xiong [35] has used Raman scattering to confirm the existence of the SO phonon modes. By microscopic approach [36,37] based on ab-initio microscopic force constants, Rossi [38,39] has found phonon modes with interface character along one or both of the in-plane directions, the latter including modes with maxima at the edges of rectangular quantum wire. Under the DC model, Stroscio [40] and Kim [41] have derived the confined LO and SO (IO) phonon modes of rectangular quantum wire, but the study did not obtain a complete description of the CO phonon modes. By means of a fully numerical treatment under the DC model and an integral equation, Knipp and Reinecke [9] have found the CO phonon modes, but they did not provide the explicit formulations of CO and EO phonon modes. In this Letter, we propose the explicit formulations for IO–propagating (IO–PR) and

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IO–IO hybrid phonon modes as well as corresponding interactions with electrons in rectangular quantum wire under the DC model. The results of numerical calculation show that these hybrid phonon modes contain CO and EO phonon modes. By the theoretical scheme of rectangular quantum wire, we derive the IO–IO–PR and IO–PR–PR hybrid phonon modes as well as corresponding interactions with electrons in rectangular quantum dot.

The Letter is organized as follows: In Section 2, we derive the IO–PR (yIO–xPR and xIO–yPR) and IO–IO hybrid phonon modes and the corresponding Fröhlich electron–phonon interaction Hamiltonian of the rectangular quantum wire. In Section 3, we deduce the IO–IO–PR (zIO–yIO–xPR, yIO–xIO–zPR and xIO–zIO–yPR) and IO–PR–PR hybrid phonon modes (zIO–yPR–xPR, yIO–xPR-zPR and xIO–zPR–yPR) and the corresponding Fröhlich electron–phonon interaction Hamiltonian of the rectangular quantum dot. In Section 4, the numerical results for two-dimensional and three-dimensional profiles of phonon potential are given and discussed. The potential applications of these results are also discussed.

2. The IO phonon modes of rectangular quantum wire

Let us consider a rectangular quantum wire of polar semiconductors embedded in a nonpolar matrix, bounded by $\pm a$ and $\pm b$ in the x and y directions, respectively. The z axis is set to along the length of quantum wire. The quantum wire and region surrounding quantum wire are taken to have dielectric constants ε_1 and ε_2, respectively, which are assumed to be isotropic. Under the DC model, we start with the electrostatic equations

$$\mathbf{D} = \varepsilon \mathbf{E} = \mathbf{E} + 4\pi \mathbf{P}, \tag{1}$$

$$\mathbf{E} = -\nabla \phi(\mathbf{r}), \tag{2}$$

$$\nabla \cdot \mathbf{D} = 4\pi \rho_0(\mathbf{r}), \tag{3}$$

where $\mathbf{D}$, $\mathbf{E}$, $\mathbf{P}$ and ϕ are the electric displacement, electric field strength, electric polarization density, and electric potential, respectively. ρ_0 is the free charge density and ε is the dielectric constant. For free oscillation, the charge density $\rho_0(\mathbf{r}) = 0$, so we get the following equation

$$\varepsilon \nabla^2 \phi(\mathbf{r}) = 0. \tag{4}$$

There are two possible solutions for Eq. (4), one of which is

$$\varepsilon(\omega) = 0, \tag{5}$$

the other is

$$\nabla^2 \phi(\mathbf{r}) = 0. \tag{6}$$

The first solution (Eq. (5)) describes the confined bulklike LO phonon modes, which have been given previously [40]. In this Letter, we focus on the second solution (Eq. (6)), which describes the IO phonon modes. Since this system is translationally invariant in the z direction, the electrostatic potential (phonon potential) describing the optical phonon modes may be taken as

$$\phi(\mathbf{r}) = \phi(x, y) e^{ik_z z} \tag{7}$$

where the k_z is the phonon wave vector in the z direction.

Substituting Eq. (7) into Eq. (6), we can obtain

$$\left[\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) - k_z^2\right]\phi(x, y) = 0. \tag{8}$$

Assuming the x and y dependent potentials to be separable, it follows that

$$\frac{1}{\phi(x)}\frac{d^2\phi(x)}{dx^2} + \frac{1}{\phi(y)}\frac{d^2\phi(y)}{dy^2} - k_z^2 = 0 \tag{9}$$

or

$$\alpha^2 + \beta^2 - k_z^2 = 0 \tag{10}$$

where $\phi(x, y) = \phi(x)\phi(y), \phi(x)$ satisfies

$$\frac{d^2\phi(x)}{dx^2} = \alpha^2 \phi(x) \tag{11}$$

and $\phi(y)$ satisfies

$$\frac{d^2\phi(y)}{dx^2} = \beta^2 \phi(y). \tag{12}$$

Since the operators $d^2/(dx^2)$ and $d^2/(dy^2)$ are Hermitian, the α^2 and β^2 must be real. So, the α and β can be either purely imaginary or purely real. When α (β) is purely imaginary, the optical modes (oscillating waves) propagate in the interior and exterior regions along the x (y) direction. We call the optical modes along the x (y) direction as PR optical phonon modes, which are similar to the PR modes in wurtzite-type heterostructures [25], quantum wells [27], superlattices [28]. When α (β) is purely real, the optical modes (decaying wave) amplitude decays exponentially in exterior regions along the x (y) direction, which are the IO modes. According to Eq. (10), there are two types (three branches) of IO phonon modes: the IO–PR (yIO–xPR and xIO–yPR) and IO–IO hybrid phonon modes.