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Polar optical phonons in core–shell semiconductor nanowires

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H I G H L I G H T S

- We obtain phonon modes for GaAs–GaP core–shell nanowires within a continuum model.
- We report a basis of functions for the space of solutions of the used model.
- Inclusion of strain produces an upwards/downwards shift of core/shell modes.

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We obtain the long-wavelength polar optical vibrational modes of semiconductor core–shell nanowires by means of a phenomenological continuum model. A basis for the space of solutions is derived, and by applying the appropriate boundary conditions, the transcendental equations for the coupled and uncoupled modes are attained. Our results are applied to the study of the GaAs–GaP core–shell nanowire, for which we calculate numerically the polar optical modes, analyzing the role of strain in the vibrational properties of this nanosystem.

1. Introduction

The study of semiconductor nanowires is of the utmost importance for the progress of the design and fabrication of novel devices and the investigation of fundamental phenomena. The development of growth techniques has allowed for the fabrication of high quality systems. Among these, the core–shell architecture is of great interest [1]: a cylindrical core of a semiconductor material is surrounded by a shell of a different semiconductor, usually with a larger bandgap. In this way, it provides a means of removing surface states and separating the carriers, or as a waveguide or cavity for optoelectronic applications. Furthermore, if the core and shell materials are grown with a lattice mismatch, the strain can be employed as an additional degree of freedom for band structure engineering. These particular systems have been synthesized employing different pairs of core–shell materials, such as GaAs–GaAsP [2], InAs–GaAs [3], GaN–GaP [4], GaP–GaN [4], GaAs–GaP [5], AlN–GaN [6], GaAsP–GaP [7], GaAs–AlGaAs [8], and CdSe/CdS [9], among others. A great variety of applications for these core–shell nanowires have appeared, for instance, nanowire lasers [2], nanowire nanosensors [10,11], photovoltaic devices [12] and light emission diodes [13], to name a few.

Polar optical phonons are of great interest for the spectroscopic characterization of core–shell nanowires of compound semiconductors. Raman scattering provides information on the phonon frequencies, which can be related to the strain in the core and the shell of the nanowires. However, in spite of its importance for their spectroscopic characterization, up to our knowledge, only a few calculations of interface modes in GaN/AlN core–shell nanowires have been reported recently, mainly obtained by means of a macroscopic dielectric model [14].

In this work we address this issue, employing a phenomenological continuum model for polar optical phonons in the long-wave limit in a cylindrical core–shell geometry. Indeed, polar optical oscillations have been successfully studied for different nanostructures applying a long-wavelength approximation and based on different continuum approaches; see, for example, Refs. [15–17] and references therein. In particular, oscillations in

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cylindrical systems have been studied in Refs. [18–20], but only for solid nanowires made of a single material, and in some cases neglecting the dispersion along the nanowire axis.

In order to study polar phonons in core–shell nanowires, we follow the approach employed for other geometries, as outlined in Refs. [15,20], and originally exposed in Ref. [21]. This phenomenological continuum model (PCM) takes into account the coupled electro-mechanical character of the vibrations without making any simplifying assumptions. From the prior experience in quasi-two-dimensional [15] and quasi-zero-dimensional systems, [22] as it was shown in Refs. [21,23,24], we do know that no further hypotheses as to the electromechanical coupling should be made when searching for linearly independent solutions in these quasi-one-dimensional structures. Some previous work following this approach has been made for cylindrical geometries [20], albeit for simple (i.e., solid and with only one material) nanowires and without considering the dependence on the axial coordinate. Here we generalize this work, considering all types of polar oscillation modes in core–shell nanowires. To this end we focus in obtaining a basis function with cylindrical symmetry, taking into account the possible angular and axial dependence the modes may have. We apply the appropriate boundary conditions for core–shell modes to a general solution, given by a linear combination of the basis functions. As we concentrate in materials with very different bulk values of their mechanical parameters, we can impose a total confinement of the mechanical components. This condition leads to the mixing of the different modes. Indeed, phonon modes of mixed nature are obtained and may display predominant longitudinal optical (*LO*), transverse optical (*TO*) or interface (*I*) profiles in the different regions of the vibrational spectra. We analyze the character of the phonon modes, and give detailed numerical results for one particular case, namely, the GaAs–GaP core–shell nanowire.

The paper is organized as follows: In Section 2 we present the fundamental equations which describe the polar oscillation modes, discussing their physical meaning and obtaining a basis for the cylindrical geometry. Section 3 explains the obtention of the polar optical modes in core–shell nanowires by applying the appropriate boundary conditions. The solution for the interface optical modes for the core–shell nanowires with cylindrical cross section in the framework of the dielectric continuum model is presented in Section 4. Section 5 discusses the inclusion of strain effects in our model. In Section 6 the results corresponding to a particular example, the GaAs–GaP core–shell nanowire, are presented. In Section 7 we draw our conclusions.

2. The phenomenological continuum model in cylindrical coordinates

We briefly recall here the formalism of the PCM employed in this work. Following the procedure developed in Refs. [21,23,24], the fundamental equations of motion which include the bulk phonon dispersion are given by

$$\rho_m(\omega^2-\omega_{TO}^2)\vec{u}=\rho_m\beta_L^2\nabla(\nabla\cdot\vec{u})-\rho_m\beta_T^2\nabla\times\nabla\times\vec{u}+\alpha\nabla\varphi, \quad (1)$$

and

$$\nabla^2\varphi=\frac{4\pi\alpha}{\varepsilon_\infty}\nabla\cdot\vec{u}, \quad (2)$$

with the parameter α defined as

$$\alpha^2=\frac{(\varepsilon_0-\varepsilon_\infty)\rho_m\omega_{TO}^2}{4\pi}. \quad (3)$$

In these expressions, ω_{TO} is the transversal bulk frequency at the Γ point, ρ_m is the reduced mass density, β_L (β_T) describes the

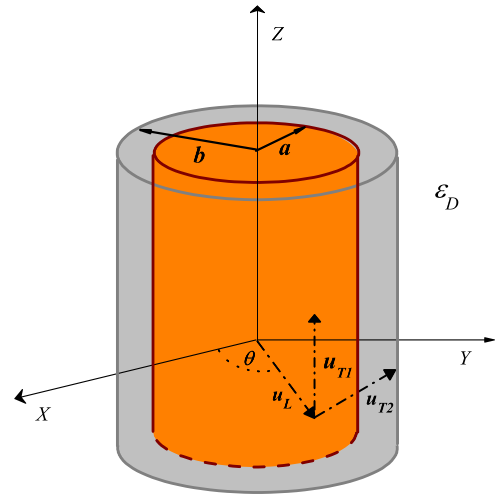

Fig. 1. Schematic representation of the capped wire system under study. In our case, the material in the core is GaAs and GaP in the shell. a (b) is the core (shell) radius. Vibrational phonon amplitudes u_L, u_{T1}, and u_{T2} are indicated. The effect associated to the embedding matrix on the vibrational modes is characterized by an outer dielectric constant ε_D.

quadratic dispersion of the *LO* (*TO*)-bulk phonon dispersion of the optical modes in the long-wave limit, and ε_0 (ε_∞) is the static (high frequency) dielectric constant. The relative mechanical displacement of the ions is represented by $\vec{u}$ and the electric potential due to the polar character of the vibrations is denoted by φ. In this model the equations are treated in the quasi-stationary approximation so a harmonic time dependence is considered for all the involved quantities.

Eqs. (1) and (2) represent a system of four coupled partial differential equations which describe the confined polar optical phonons in each region of the semiconductor heterostructure. In this particular case, hybrid core–shell cylindrical nanowires consist of a material "*s*" grown on a core structure of material "*c*" , and the medium properties are considered piecewise, as depicted in Fig. 1. Furthermore, the nanowire is embedded in a host material, which is typically a silicate matrix or an organic polymeric compound.

We model the core–shell nanowire as an infinite cylinder of circular cross section with radius a, dressed by a cylindrical shell of another material with external radius b (see Fig. 1). The wire is embedded in a host material uncoupled to the oscillations of the nanowire, characterized by its dielectric constant ε_D.

In order to find a general solution for the oscillations of the nanowire, we have to find a basis for the solutions in each region. With this purpose, we follow the method of the potentials described in detail in the book by Morse and Feshbach [25] that we sketch briefly.

First, we introduce the auxiliary potentials $\vec{\Gamma}$ and Λ such that

$$\vec{\Gamma}=\nabla\times\vec{u} \quad \text{and} \quad \Lambda=\nabla\cdot\vec{u}. \quad (4)$$

Taking the curl and the divergence of Eq. (1), we obtain the following new equations for the potentials:

$$\nabla^2\vec{\Gamma}+Q_T^2\vec{\Gamma}=\vec{0}, \quad (5)$$

$$\nabla^2\Lambda+Q_L^2\Lambda=0, \quad (6)$$

with Q_T, Q_L given by

$$Q_T^2=\frac{\omega_{TO}^2-\omega^2}{\beta_T^2},$$