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Properties of interface phonon spectra in complicated cylindrical nanosystems

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The spectra of two types of interface phonons (top and side optical) are studied within the framework of dielectric continuum model for combined nanoheterosystems consisting of semiconductor cylindrical quantum dots inside the cylindrical quantum wire placed into dielectric or semiconductor medium. The dependencies of both types of interface phonon energies on the quasiwave numbers and geometric parameters of nanosystem are calculated and analysed.

Key words: *nanoheterosystem, phonon, quasiwave number, energy*

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1. Introduction

For the past few years there has been observed a rapid development of experimental and theoretical investigations not only of the nanoscale objects (quantum dots, wires and wells) but their spatial combinations as well [1]. The experimental treatment of the quantum objects exhibiting the variety of shapes such as sphere, cylinder or rectangle, have caused the creation of rather complicated combined constructions having dimensions within a few nanometers. There unique properties are used in different modern devices, i.e. quantum computers [2,3].

The theory of quasiparticles spectra in single quantum dots, wires and wells embedded into the dielectric or semiconductor external medium have been established for the past few years [4–6] within the effective mass approximation and rectangular potentials for the electron, hole, exciton and dielectric continuum model for the phonons. The investigations of physical properties, such as carrier relaxation and transportation, linear and non-linear optical characteristics of quantum dots, the interaction between quasiparticles and phonons are carried out both experimentally and theoretically.

The complicated nanoconstructions created experimentally, contain different spatial combinations of quantum dots, wires and wells [1]. These objects are actively studied theoretically, in spite of the mathematical difficulties arising due to the complicated fitting conditions for the wave functions of quasiparticles and polarization potentials of free vibrations.

It is obvious that in order to profoundly understand the properties of any nanoconstruction one has to perform a precise description of all optical phonon modes, study the quasiparticles spectra and establish the Hamiltonian of interaction between quasiparticles and phonons. Wai-Sang Li and Chuan-Yu Chen [7] have studied a cylindrical quantum dot in vacuum and derived confined LO phonons and two types of interface phonon modes with their eigenfunctions using the dielectric continuum approach. The analytical investigations of phonon spectra in three cylindrical quantum dots in the cylindrical quantum wire placed into the semiconductor external medium were performed in [8]. Both references present only the analytical derivations without any numeric calculations and analysis of phonon spectra for the specific nanoconstructions.

In this paper the energies and dispersion laws of interface vibrations are studied for the two types of a combined nanoheterosystem consisting of semiconductor cylindrical quantum dot embed-

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ded into the cylindrical semiconductor quantum wire placed into the semiconductor or dielectric external medium (water). The phonon spectrum is treated within the framework of the dielectric continuum model widely applied for low-dimensional crystal structures [6–9] and the results of which are in good correlation with the experimental data.

2. Theory of interface phonon spectra

The interface phonon spectra are studied for two types of a combined nanosystem consisting of a semiconductor cylindrical quantum dot (HgS "0") embedded into the cylindrical quantum wire (CdS "1") placed into the semiconductor (ZnS "2", figure 1a) or dielectric (water "2" , figure 1b) outer medium. The radii of a quantum dot (QD) and quantum wire (QW) are considered to be equal (ρ_0), the QD height is Δ_0 and the dielectric constant of every i-th part of nanosystem is assumed to be:

$$\varepsilon_i(\omega) = \varepsilon_{i\infty}\frac{\omega^2-\omega_{Li}^2}{\omega^2-\omega_{Ti}^2}, \qquad i = 0,1,2,\ldots, \tag{1}$$

where $\varepsilon_{i\infty}$ is a high frequency dielectric constant, ω_{Li} and ω_{Ti} are the frequencies of longitudinal and transversal optical phonons of the respective bulk crystals. In case the external medium is dielectric, $\varepsilon_2 = \varepsilon_d = 1.78$. The phonon spectrum for such a system is obtained within the dielectric continuum model combining the electrostatic equations [6] and getting

$$\varepsilon_i(\omega)\nabla^2\Phi(\vec{r}) = 0, \tag{2}$$

where $\Phi(\vec{r})$ is the potential of phonon polarization field. It is clear that there are two possible solutions to this equation defining the spectra of confined and interface phonons which are observed hereafter. It is well known that the first solution of equation (2) proves that the frequencies of confined phonons are equal to the frequencies of longitudinal phonons of the corresponding composing parts of a nanosystem [6–8]. The second solution: $\Delta\Phi(\vec{r}) = 0$, determines the spectra of interface phonons. According to the cylindrical symmetry of the system, the polarization potential can be chosen as

$$\Phi(\vec{r}) = \varphi(\rho)F(z)e^{im\varphi}. \tag{3}$$

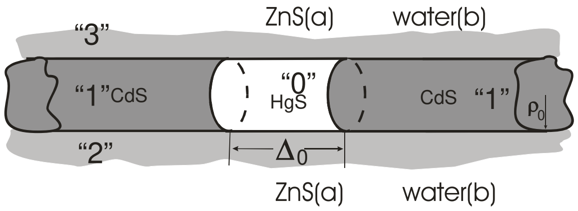

Figure 1. a,b. Geometrical scheme of combined nanosystem.

Obviously, the solutions for the two planes are quite different from the solutions at the side walls. Depending on the boundary conditions for the $F(z)$ and $\varphi(\rho)$ functions ([7]) there are two types of interface phonon modes: top surface optical (TSO) modes with the amplitude decreasing away from the two planes and side surface optical (SSO) modes with the amplitude decreasing away from the side walls.

Top surface optical (TSO) modes

It is clear that for the TSO modes, the $\varphi(\rho)$ function should describe the non-decaying potential in the plane perpendicular to the OZ axis and decaying $F(z)$ along this axis. Consequently,

$$\varphi(\rho) = \begin{cases} J_m(q\rho), & \rho \leqslant \rho_0\,, \\ N_m(q\rho), & \rho > \rho_0\,, \end{cases} \tag{4}$$

$$F(z)=\begin{cases} B_0^{+}\operatorname{ch}(qz)+B_0^{-}\operatorname{sh}(qz), & |z|\leqslant \Delta_0/2\,,\\ B_1 e^{-qz}, & |z|>\Delta_0\,. \end{cases} \tag{5}$$

From the boundary conditions for the polarization potential and normal terms of electric displacement at $z=\pm\Delta_0/2$, there are obtained antisymmetric (ω_-) or symmetric (ω_+) TSO modes. As a result, one can get a system of two equations

$$\begin{cases} B_0^{\pm}\mathrm{Csh}^{\pm}(qz)=B_1 e^{-qz}\,,\\ \pm\varepsilon_0 B_0^{\pm}\mathrm{Sch}^{\pm}(qz)=-\varepsilon_1 B_1 e^{-qz}, \end{cases} \tag{6}$$

where

$$\mathrm{Csh}^{\pm}(qz)=\begin{cases} \mathrm{Ch}(qz),\text{“ + ”}\,,\\ \mathrm{Sh}(qz),\text{“ − ”}\,, \end{cases}\qquad \mathrm{Sch}^{\pm}(qz)=\begin{cases} \mathrm{Sh}(qz),\text{“ + ”}\,,\\ \mathrm{Ch}(qz),\text{“ − ”}\,. \end{cases} \tag{7}$$

The condition of non-trivial solutions of equations (6) leads to the equation fixing the frequencies of TSO phonons

$$g_2\omega^4-g_1\omega^2+g_0=0, \tag{8}$$

where

$$\begin{aligned} g_0 &= \alpha\omega_{T1}^2\omega_{L0}^2-\beta\omega_{T0}^2\omega_{L1}^2, \qquad g_2=\alpha-\beta,\\ g_1 &= \alpha(\omega_{T1}^2+\omega_{L0}^2)-\beta(\omega_{T0}^2+\omega_{L1}^2),\\ \alpha &= \pm\frac{\mathrm{Sch}^{\pm}(gz)}{\mathrm{Csh}^{\pm}(gz)}\,, \qquad \beta=-\frac{\varepsilon_{1\infty}}{\varepsilon_{0\infty}}\,. \end{aligned} \tag{9}$$

We are going to discuss the results of computer calculations performed for the specific nanosystem hereafter.

Side surface optical (SSO) modes

For the SSO modes the $F(z)$ function should describe the non-decaying potential along the OZ axis and decaying $\varphi(\rho)$ in the perpendicular plane. Thus, it is convenient to take as follows:

$$\Phi(\vec r)=\begin{cases} I_m(k\rho)\,(D^{+}\cos(kz)+D^{-}\sin(kz))\,\mathrm{e}^{im\varphi}, & \rho\leqslant\rho_0\\ K_m(k\rho)\,(C^{+}\cos(kz)+C^{-}\sin(kz))\,\mathrm{e}^{im\varphi}, & \rho>\rho_0 \end{cases}\,. \tag{10}$$

The unknown coefficients are found during the second quantization of the phonon field, $I_m(k\rho)$ and $K_m(k\rho)$ is the m-th order modified Bessel functions of the first and second type. The frequencies of SSO phonons are also determined by the boundary conditions for the polarization potential and normal terms of electric displacement at the condition $\rho=\rho_0$. The ratio of the respective equations gives the transcendental equation

$$\varepsilon_i\frac{I_m'(k\rho_0)}{I_m(k\rho_0)}=\varepsilon_2\frac{K_m'(k\rho_0)}{K_m(k\rho_0)}\,, \qquad i=0,1. \tag{11}$$

Solving the latter we get the dispersion equation for the frequencies of SSO modes.

When the quantum dot, wire and outer medium are all semiconductors, the frequencies are fixed by the expression

$$\omega_i(k\rho_0)=\sqrt{\frac{-b_i\pm\sqrt{b_i^2-4a_ic_i}}{2a_i}}, \tag{12}$$

where

$$\begin{aligned} a_i &= \varepsilon_{i\infty}-\varepsilon_{2\infty}P(k\rho_0),\\ b_i &= \varepsilon_{2\infty}P(k\rho_0)(\omega_{Ti}^2-\omega_{L2}^2)-\varepsilon_{i\infty}(\omega_{T2}^2-\omega_{Li}^2),\\ c_i &= \varepsilon_{i\infty}\omega_{Li}^2\omega_{T2}^2-\varepsilon_{2\infty}P(k\rho_0)\omega_{L2}^2\omega_{Ti}^2\,,\\ P(k\rho_0) &= \frac{I_m(k\rho_0)}{K_m(k\rho_0)}\times\frac{mK_m(k\rho_0)-k\rho_0K_{m+1}(k\rho_0)}{mI_m(k\rho_0)+k\rho_0I_{m+1}(k\rho_0)}\,. \end{aligned} \tag{13}$$

The expression (12) proves that there are four bands (formed over the magnetic quantum number) of SSO modes for two side walls, produced by the interfaces between two semiconductor media (dot/outer medium and wire/outer medium).

When the quantum dot and wire are semiconductors and the outer medium is dielectric, the frequencies of SSO phonons for the i-th part of nanosystem are fixed by the expression

$$\omega_i(k\rho_0) = \sqrt{\frac{\varepsilon_d \omega_{Ti}^2 P(k\rho_0) - \omega_{Li}^2 \varepsilon_{i\infty}}{\varepsilon_d P(k\rho_0) - \varepsilon_{i\infty}}}\,. \tag{14}$$

The expression (14) proves that there are two bands of SSO modes for every side wall, produced by the interface between semiconductor and dielectric media (dot/outer medium and wire/outer medium). The results of the numeric calculations for the particular system are also analysed hereafter.

3. Discussion of the results

The results of the computer calculations of the TSO and SSO phonon energies are presented in figures 2–4. The numeric calculations were performed for the cylindrical nanosystems CdS/HgS/CdS placed into ZnS outer medium or into the water (figure 1a,b). The choice of these specific nanosystems is conditioned, on the one hand, by the dielectric continuum model and, on the other hand, by the requirements of the effective mass approximation and rectangular potentials for the quasiparticles (the close magnitudes of the lattice constants). The latter are important for the possible future investigations of interaction between quasiparticles and phonons.

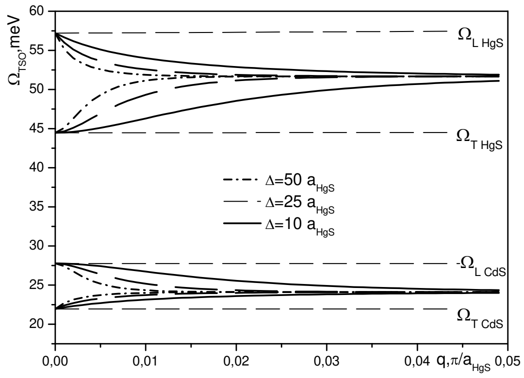

Figure 2. Dependence of TSO phonon energy on the quasiwave number for the different thickness of HgS QD ($\Delta_0 = 10a_{\mathrm{HgS}}, 25a_{\mathrm{HgS}}, 50a_{\mathrm{HgS}}$).

It should to be mentioned that the behavior of the interface phonon spectra depends on the geometrical parameters of a nanosystem and on the type of vibrations (SSO or TSO) but the energies of all these phonon modes are always located between the energies of LO and TO phonons of the respective bulk crystals ($\Omega_{L_{\mathrm{CdS}}}$, $\Omega_{T_{\mathrm{CdS}}}$, $\Omega_{L_{\mathrm{ZnS}}}$, $\Omega_{T_{\mathrm{ZnS}}}$, and $\Omega_{L_{\mathrm{HgS}}}$, $\Omega_{T_{\mathrm{HgS}}}$ shown in the figures by dashed lines).

In figure 2 there is shown the evolution of TSO phonon energy spectra as a function of quasiwave number q (in units of lattice constant of HgS crystal) for different thicknesses ($\Delta_0 = 10a_{\mathrm{HgS}}, 25a_{\mathrm{HgS}}, 50a_{\mathrm{HgS}}$) of QD HgS. From the figure it is clear that there are four modes of TSO vibrations: two vibrations with positive (symmetric) and two vibrations with negative (antisymmetric) dispersion shown by the respective curves. They are caused by the presence of two plane interfaces between QD HgS and QW CdS. The dependence on the quasiwave number is essential only for the small magnitudes of the latter and then the curves are smoothly tending to saturation. This fact makes it easier to study the interaction between quasiparticles and phonons that can be assumed as dispersionless. At a fixed quantum number, the energies of TSO phonons are bigger for the bigger thickness of HgS QD for the modes with a positive dispersion and smaller for the modes with negative dispersion.

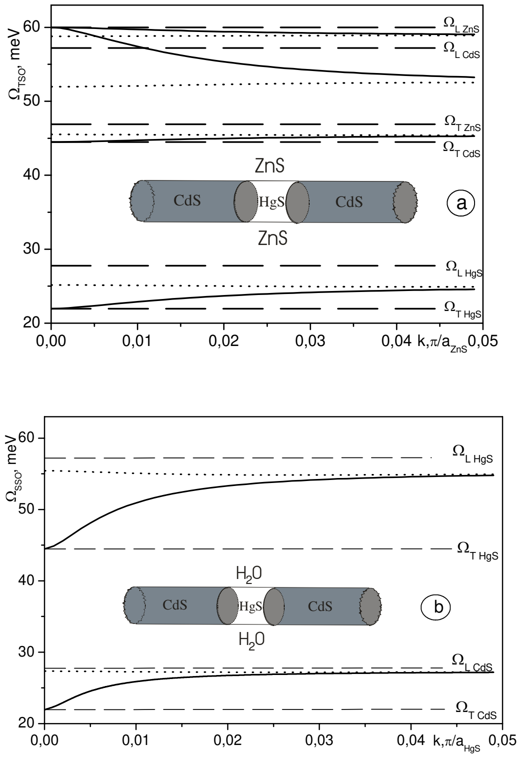

Figure 3. Dependence of SSO phonon energy on the quasiwave number for magnetic quantum number $m = 0(-), m = 1(\ldots)$.

In figure 3a,b there is shown the dependence of SSO phonon energies on the quasiwave number for two nanoconstructions: CdS/HgS/CdS placed into ZnS outer medium (figure 3a) and CdS/HgS/CdS placed into the water (figure 3b). The difference is obvious because, as it is proved by the formulas (12)–(14), in figure 3a, one can see four bands of SSO phonon energies: two of them arise due to the side interface HgS/ZnS and the other two arise due to the interface CgS/ZnS. In figure 3b there are two bands of SSO phonon energies: one band is produced by the interface HgS/H_2O and the other is produced by the interface CdS/H_2O. The bands are formed over the magnetic quantum number (m). Computer calculations show that the energies of SSO phonons

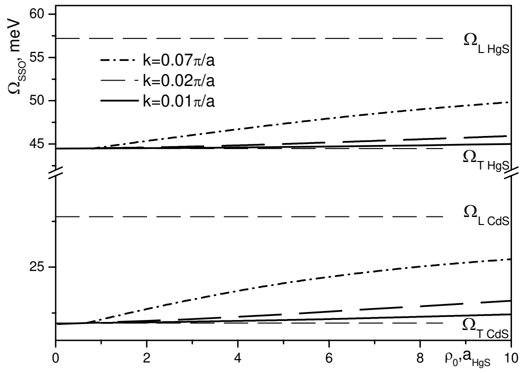

Figure 4. Dependence of SSO phonon energy on the radius of nanoconstruction.

with $m > 1$ are almost the same as for the energy with $m = 1$, since in the figure there are shown the dependences only for $m = 0$ and $m = 1$. The dispersion of the energies on the quasiwave number is noticeable only for the small magnitudes of the latter and then the curves are also tending to saturation.

In figure 4 there is shown the dependence of SSO phonon energies on the radius of nanoconstruction (ρ_0) for different magnitudes of the quasiwave number k. The figure proves that the dependence on the radius is rather weak. The SSO modes also form the respective bands over the magnetic number but in the figure there are presented the results calculated only for $m = 0$ in order not to overload the figure because the dependencies are quite similar to the ones shown in figure 3a,b.

The obtained frequencies of TSO and SSO phonons and their dispersion laws will be further used for the study of interaction between quasiparticles and these types of vibrations in the combined cylindrical nanosystems.

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Властивості спектру інтерфейсних фононів у складних циліндричних наносистемах

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У межах моделі діелектричного континууму вивчаються спектри двох типів інтерфейсних фононів (вершинних і бічних оптичних), що існують у комбінованій наногетеросистемі, яка складається з напівпровідникової квантової точки всередині циліндричного квантового дроту, поміщеного у діелектричне або напівпровідникове середовище. Отримано і проаналізовано залежності енергій обох типів інтерфейсних фононів від квазіхвильових чисел і геометричних параметрів наносистем.

Ключові слова: *наносистема, фонон, квазіхвильове число, енергія*

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