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Spectrum of confined and interface phonons in complicated cylindrical nanoheterosystem placed into the plane quantum well in water

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The energy spectra of all types of free vibrations existing in combined nanoheterosystem consisting of cylindrical semiconductor quantum dot, semiconductor quantum ring embedded into the quantum well placed in water are studied in the framework of dielectric continuum model. It is shown that depending on the boundary conditions for the potentials of polarization fields there are two types of interface phonon modes: top (bottom) surface optical (TSO) modes and side surface optical (SSO) modes.

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1. Introduction

The theory of quasiparticle (electron, hole, exciton) spectra in different combined nanoheterosystems have been rapidly developed recently [1, 2, 3]. It is caused by the unique perspectives of their utilization in the devices of modern semiconductor nanoelectronics [4].

Since, in ref. [1,2] the electron, hole and exciton spectra in opened combined nanoheterosystems were investigated in details. It was shown that the quasiparticle in such system is characterized by quasistationary states with the finite life time. Therefore the energy loss of quasiparticles (electrons, holes) can be caused not only by their recombination accompanied by the radiation of photons but also by the ability of quasiparticles to tunnel through the finite potential barrier with their further movement to the infinity.

As far as we know, there is no the strait theory of interaction between quasiparticles and polarization fields in the combined nanoheterosystems yet. Nevertheless, such interaction, obviously, influences the energy spectra of quasiparticles, that is to be experimentally observed at the luminescence spectra.

It is convenient to study the interaction between quasiparticles and phonons within the Green functions method using the Feinman diagram technique [5]. But, at first, it is necessary to obtain the energy spectra of quasiparticles and potentials of polarization fields arising in such systems.

In ref. [3] there were investigated all types of phonon modes existing in the single combined nanoheterosystem consisting of semiconductor quantum dot, embedded into the semiconductor quantum wire. Here it was established for the first time that there are two types of interface phonon modes: top surface optical and side surface optical modes.

In this paper we investigated in details the energy spectra of all types of free vibrations observed in the combined nanoheterosystem consisting of cylindrical semiconductor quantum dot (QD), semiconductor quantum ring embedded into the quantum well (QW), placed into the water. The research is performed within the dielectric continuum model, the results of which are in good correlation to the experimental data obtained for the simplest systems [6].

2. Theory of confined and interface phonon spectra

The combined nanoheterosystem (fig. 1) consisting of cylindrical semiconductor quantum dot with the height h_0 and radius ρ_0 (*HgS*, "0"), semiconductor quantum ring with the thickness Δ (*CdS*, "1"), embedded into the quantum well (*HgS*, "2"), placed into the dielectric medium (*water*, "3") is under research.

The dielectric constants of every i th part of nanosystem is assumed as known

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

where $\varepsilon_{i\infty}$ - the high frequency dielectric constant, ω_{Li} and ω_{Ti} - the frequencies of longitudinal and transversal optical phonons of the respective bulk analogues of nanocrystals, $\varepsilon_3 = 1,78$ [7].

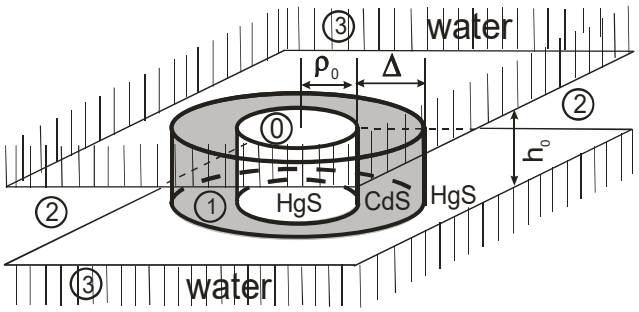

Fig.1. Geometrical scheme of combined nanoheterosystem.

According to the dielectric continuum model, the polarization field of the system is defined by the Maxwell equations for the media

$$\begin{cases} \boldsymbol{D} = \varepsilon(\boldsymbol{r},\omega)\boldsymbol{E} = \boldsymbol{E} + 4\pi\boldsymbol{P} \\ \boldsymbol{E} = -\nabla\Phi \\ \nabla\boldsymbol{D} = 0 \end{cases}, \qquad (2)$$

where $\boldsymbol{P}$ and $\boldsymbol{D}$ - electric polarization and displacement, respectively, $\Phi(\boldsymbol{r})$ - potential of polarization field. From the system of equations (2) it is obtained the equation

$$\varepsilon(\boldsymbol{r},\omega)\,\Delta\Phi(\boldsymbol{r}) = 0, \qquad (3)$$

the solutions of which determine the spectra of vibrations for the nanosystem.

2.1. Confined phonons

From the condition

$$\varepsilon(\boldsymbol{r},\omega) = 0, \qquad \Delta\Phi(\boldsymbol{r}) \neq 0, \qquad (4)$$

it is obtained the spectrum of confined optical phonons. Analysis of eqs. (4) with eq.(1) proves that the frequencies of confined phonons are equal to the corresponding frequencies of confined phonons for the respective bulk crystals and, since, the energies of the confined phonons are

$$\Omega_{Li} = \mathrm{h}\,\omega_{Li}. \qquad (5)$$

Taking into the account the cylindrical symmetry of the problem, the polarization field of confined phonons of nanosystem i -th part is chosen in the form

$$\Phi_{Li}(\boldsymbol{r}) = \sum_{q_\parallel, q_\perp, m} \Phi_m^i(q_\parallel, q_\perp) \begin{Bmatrix} \cos(q_\parallel z) \\ \sin(q_\parallel z) \end{Bmatrix} e^{im\varphi} \left[A_i J_m(q_\perp\rho) + B_i N_m(q_\perp\rho)\right], \qquad (6)$$

where $J_m(q_\perp\rho)$, $N_m(q_\perp\rho)$ - Bessel functions, $q_\parallel, q_\perp$ - axial and radial quasiwave numbers, m - magnetic quantum number. The unknown coefficients A_i, B_i, $\Phi_m^i(q_\parallel, q_\perp)$ are obtained during the second quantization of the phonon field.

2.2. Interface phonons

The other solution of eq. (3)

$$\varepsilon(\boldsymbol{r},\omega) \neq 0, \quad \Delta\Phi(\boldsymbol{r}) = 0 \qquad (7)$$

defines the spectrum and potential of polarization field for the interface phonons in nanosystem.

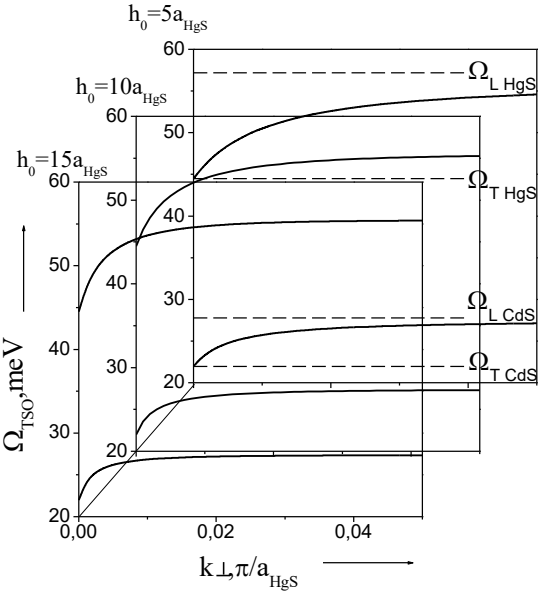

Fig. 2. Dependences of TSO phonon energies (Ω_{TSO}) on the radial quasiwave number ($k_\perp$) for the different values of QD height (h_0).

Due to the symmetry of the problem, the solution of Laplace's equation (7) mustbe taken in the form

$$\Phi(\boldsymbol{r}) = \varphi(\rho)F(z)e^{im\varphi}. \qquad (8)$$

Depending on the fitting conditions for the functions $\varphi(\rho)$ and $F(z)$ there are two types of interface phonon modes: top (bottom) surface optical (TSO) modes, whose amplitude decreases away from the interface of quantum well $|z| = h_0/2$, and side surface optical (SSO) modes, whose amplitude decreases away from the side walls at $\rho = \rho_0$ i $\rho = \rho_0 + \Delta$.

a) TSO phonons

It is obvious that for the TSO phonons $\varphi(\rho)$ function is to describe the non decaying potential in the plane perpendicular to the axis of QD. Thus,

$$\Phi_{TSO}(\boldsymbol{r}) = J_m(k_\perp \rho) e^{im\varphi} \begin{cases} \begin{cases} C^+_{k_\perp} ch(k_\perp z) \\ C^-_{k_\perp} sh(k_\perp z) \end{cases}, & z \le h_0/2 \\ D_{k_\perp} e^{-k_\perp z}, & z > h_0/2 \end{cases} . \quad (9)$$

Using, further, the boundary conditions for the continuity of polarization potential and normal term of dielectric displacement at $z = h_0/2$, it is obtained the dispersion equation

$$\varepsilon_i(\omega) \begin{Bmatrix} th(k_\perp h_0/2) \\ cth(k_\perp h_0/2) \end{Bmatrix} = -1,78, \qquad i = 1,2 \quad (10)$$

Inserting eq.(1) into (10) one can otain the frequencies and finally the energies of TSO phonons as functions of quasiwave number $k_\perp$.

The unknown coefficients in eq.(9) are defined at the second quantization of TSO phonons.

b) SSO – phonons

For SSO – modes $F(z)$ function is to describe the non decaying potential along OZ axis and decaying $\varphi(\rho)$ in the perpendicular plane. Since,

$$\Phi_{SSO}(\boldsymbol{r}) = e^{ik_\parallel z} e^{im\varphi} \begin{cases} A^{(0)}_{k_\parallel} I_m(k_\parallel \rho), & 0 \le \rho \le \rho_0 \\ A^{(1)}_{k_\parallel} I_m(k_\parallel \rho) + B^{(1)}_{k_\parallel} K_m(k_\parallel \rho), & \rho_0 \le \rho \le \rho_0 + \Delta \\ B^{(2)}_{k_\parallel} K_m(k_\parallel \rho), & \rho > \rho_0 + \Delta \end{cases} \quad (11)$$

Here, $I_m(k_\parallel \rho)$, $K_m(k_\parallel \rho)$ - modified cylindrical Bessel functions of first and second kind. The boundary conditions for the continuity of polarization potential and normal term of dielectric displacement at $\rho = \rho_0$ and $\rho = \rho_0 + \Delta$ allow to express the unknown coefficients $B^{(2)}_{k_\parallel}, A^{(1)}_{k_\parallel}, B^{(1)}_{k_\parallel}$ through $A^{(0)}_{k_\parallel}$ and finally bring to the dispersion equation (the latter is not presented due to it is sophisticated) for the defining of SSO phonon frequencies as functions of axial quasiwave number $k_\parallel$. The coefficient $A^{(0)}_{k_\parallel}$ is also defined during the second quantization of SSO phonons field.

3. Discussion

Computer calculations of TSO and SSO phonon energies were performed for the combined nanoheterosystem (Fig. 1) with physical parameters presented in ref. [5]. The results are presented in figs.2-4. It is clear and the figures prove that the spectra of interface phonons depend on the geometrical parameters of nanoheterosystem and on the type of vibrations (SSO or TSO). But the energies of all modes of vibrations are always located between the energies of longitudinal and transversal phonons of the respective bulk crystals ($\Omega_{T\,CdS}$, $\Omega_{L\,CdS}$, $\Omega_{T\,HgS}$, $\Omega_{L\,HgS}$) shown in the figures by dash lines.

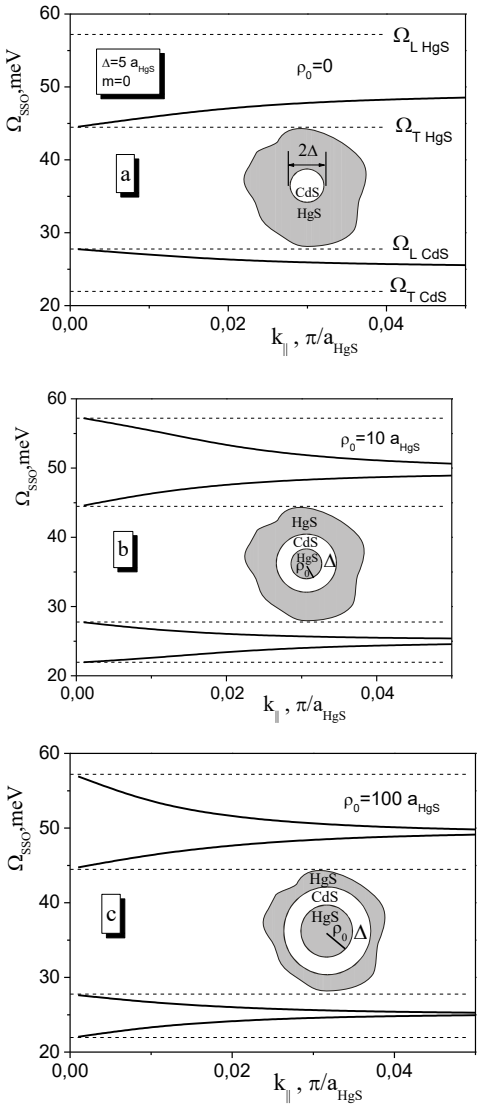

*Fig. 3. Dependences of SSO phonon energies (Ω_{SSO}) on the axial quasiwave number ($k_\parallel$) at $\Delta = 5\,a_{CdS}$, $m = 0$ for the different values of QD radius (ρ_0): $\rho_0 = 0$ **(a)**, $\rho_0 = 10\,a_{HgS}$ **(b)**, $\rho_0 = 100\,a_{HgS}$ **(c)**.*

In Fig. 2 the dependence of TSO phonons energies on the radial quasiwave number $k_\perp$ is presented for the different values of QD height (h_0). From the figure one can see two modes of TSO phonons with positive dispersion over the quasiwave number $k_\perp$. These two modes are caused by the existence of two interfaces HgS/water and CdS/water. We must note that the spectra of TSO phonon energies almost do not depend on the radius of QD (ρ_0) and on the thickness of semiconductor ring (Δ). The increasing of QD height (h_0) causes the small increasing of the dispersion over $k_\perp$ (Fig. 2).

In Fig. 3a,b,c there are presented the dependences of SSO phonon energies on the axial quasiwave number $k_{\|}$ at $\Delta = 5\,a_{CdS}$, $m = 0$ for the three values of QD radius (ρ_0): $\rho_0 = 0$ (Fig. 3a), $\rho_0 = 10\,a_{HgS}$ (Fig. 3b), $\rho_0 = 100\,a_{HgS}$ (Fig. 3c).

At $\rho_0 = 0$ there are two SSO modes with the opposite dispersions over the quasiwave number $k_{\|}$. It is clear because at $\rho_0 = 0$ one obtains the spectrum of SSO phonons in CdS QD with radius $\Delta = 5\,a_{CdS}$, embedded into HgS QW, i.e., the system with one interface CdS/HgS producing two side surface optical modes (Fig. 3a). The appearance of QD inside and increasing of its radius, causes the arising of two new SSO modes with different dispersions due to the new interface HgS/CdS between QD (HgS) and quantum ring (CdS) (Fig. 3d,c). From the figures one can see that at $\rho_0 > 100\,a_{HgS}$ there are almost no any changes in the behavior and energy values of SSO phonons. It is clear because at the big ρ_0 magnitudes the curvature of QD side surface becomes so small that the cylindrical nanosystem is transformed into the plane film with the thickness $\Delta = 5\,a_{CdS}$, embedded into the quantum well HgS.

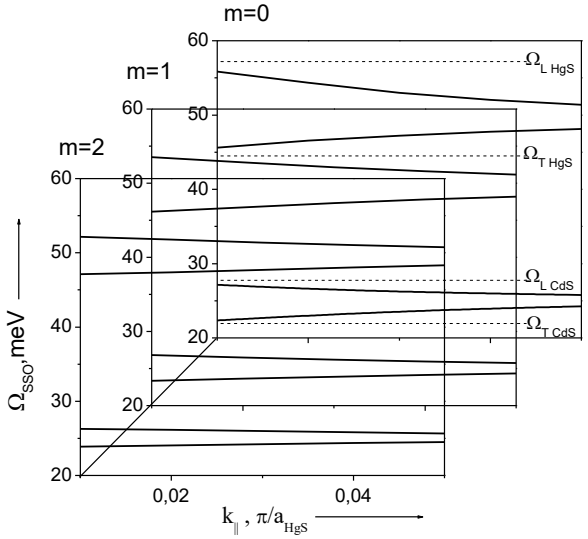

Fig. 4. Dependences of SSO phonon energies (Ω_{SSO}) on the axial quasiwave number ($k_{\|}$) at $\rho_0 = 10\,a_{HgS}$, $\Delta = 5\,a_{CdS}$ for the different values of magnetic quantum number (m): $m = 0$, $m = 1$, $m = 2$.

In Fig. 4 the evolution of SSO phonon spectrum at $\rho_0 = 10\,a_{HgS}$, $\Delta = 5\,a_{CdS}$ and different values of magnetic quantum number m: $m = 0$, $m = 1$, $m = 2$ is presented. Figure proves that the dispersion of energy over magnetic quantum number is rather small. The energies of modes with $m > 1$ are almost the same as the energies with $m = 1$. There is the infinite number of SSO modes in the system under research because the magnetic quantum number has the infinite number of values.

The energies of confined, SSO and TSO phonons obtained in the paper and their dispersion laws would be further used for the investigation of interaction between quasiparticles (electrons, holes, excitons) and these types of vibrations.

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