PHONON SPECTRA AND ELECTRON-PHONON INTERACTION IN A COMBINED CYLINDRICAL SEMICONDUCTOR NANOTUBE

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PACS 63.22.Gh, 78.67.Ch, 73.21.Hb

A theory of electron-phonon interaction in a combined cylindrical semiconductor nanotube has been developed in the framework of the effective mass model for electrons and a dielectric continuum for phonons. Analytical expressions for Hamiltonians of electron interaction with confined and interface phonons have been derived in the secondary quantization representation for electron and phonon variables. Dependences of the phonon energies and the interface phonon polarization field potential on the axial quasimomentum and the geometrical parameters of a combined nanotube fabricated on the basis of GaAs and $Al_{0.4}Ga_{0.6}As$ semiconductors have been studied.

1. Introduction

Semiconductor quantum wires have been studied both theoretically and experimentally for 20 years. The improvement of methods aimed at their growing–such as molecular-beam, gas-phase, and metal-organic epitaxy–made it possible to form not only single wires, but also the ensembles of quantum nanowires with a radial heterostructure, which are perfectly arranged in space [1, 2]. On the one hand, such a heterostructure, which is perpendicular to the quantum wire axis, can localize charge carriers in the wire core by reducing the surface scattering [3]. On the other hand, it allows the spectral parameters of major quasiparticles in the nanosystem (electrons, excitons, phonons) to be changed purposefully by varying the geometrical parameters of a heterostructure. Unique properties of quasiparticles in such systems allow them to be used as base elements in tunnel nano-diodes, nano-transistors with a high mobility of electrons, high-performance light-emitting devices, photoconverters, and nanosensors for the diagnostics of various biological and chemical compounds [4].

Intensively studied semiconductor nanotubes belong to quantum wires with a radial heterostructure. Depending on semiconductor materials that compose a heterostructure, experimenters have already created simple (with a single quantum well for an electron) [5, 6] and complex (multi-well) multilayered nanotubes [7, 8]. Simple quantum wires and nanotubes were studied theoretically in detail in works [9–11]. The cited authors developed a theory for the energy spectra of electrons, holes, and phonons and for the interaction of those quasiparticles with one another. The theory allowed them to obtain not only qualitative but also quantitative agreement with experimental data.

Theoretical researches of combined multilayered semiconductor nanotubes are at their beginning. In particular, the theory of electron and exciton energy spectra was elaborated in work [12], and their dependence on the geometrical parameters of combined nanotubes was analyzed. Today, as far as we know, there is no consistent theory for the phonon spectrum in such systems. As a result, the theory of the interaction between an electron and phonons, which are considered as one of the dissipation subsystems that should evidently affect the radiative or absorption ability of a nanotube, is also absent.

Therefore, this work aimed at constructing the theory of phonon spectra and electron-phonon interaction in combined cylindrical semiconductor nanotubes (Fig. 1). As an example, we studied the features in the main characteristics of the phonon field and their dependences

on the geometrical parameters of nanosystems based on GaAs and $Al_{0.4}Ga_{0.6}As$ semiconductors.

2. Energy Spectrum and Wave Functions of an Electron in a Combined Cylindrical Semiconductor Nanotube without regard for the Interaction with Phonons

Here, we analyze a nanosystem that is a combined cylindrical semiconductor nanotube. It consists of a quantum core wire (medium 0), a thin semiconductor layer (a barrier, medium 1), and a nanotube (medium 2), with the entire nanosystem being located in the external environment (medium 3), as is shown in Fig. 1.

The lattice constants (a_0 and a_1) and the dielectric permittivities of nanosystem components are supposed to differ weakly from each other. In addition, the nanosystem dimensions are supposed to satisfy the relation $(\rho_0, \Delta, h) > (a_0, a_1)$. Therefore, the effective mass (μ) approximation [13, 14] and the rectangular potential (U) model can be used to calculate the energy spectrum of electrons. Note that the dielectric permittivities, effective masses, and potential energy of an electron are considered to be known in every region of the combined nanotube. In the cylindrical coordinate system with the axis OZ directed along the nanosystem axis, those quantities are defined as follows:

$$\varepsilon(\rho,\,\omega) = \begin{cases} \varepsilon_0(\omega) \\ \varepsilon_1(\omega) \end{cases}, \quad \mu(\rho) = \begin{cases} \mu_0 \\ \mu_1 \end{cases},$$

$$U(\rho) = \begin{cases} 0, & 0 \le \rho \le \rho_0, \quad \rho_1 \le \rho \le \rho_2 \\ U_0, & \rho_0 \le \rho \le \rho_1, \quad \rho > \rho_2 \end{cases}. \tag{1}$$

The Hamiltonian of an electron without regard for its interaction with phonons looks like

$$\hat{H}_e(\rho,\,\varphi,\,z) = -\frac{\hbar^2}{2\mu(\rho)}\frac{\partial^2}{\partial z^2} + U(\rho) -$$

$$-\frac{\hbar^2}{2\rho}\left[\frac{\partial}{\partial\rho}\left(\frac{\rho}{\mu(\rho)}\right)\frac{\partial}{\partial\rho} + \frac{1}{\rho}\frac{\partial^2}{\partial\varphi^2}\right]. \tag{2}$$

The stationary Schrödinger equation

$$\hat{H}_e(\rho,\,\varphi,z)\,\psi(\rho,\,\varphi,z) = E\,\psi(\rho,\,\varphi,z) \tag{3}$$

can be solved exactly, so that the sought wave functions have the form

$$\Psi_{m\,k}(\mathbf{r}) = \frac{1}{\sqrt{2\pi\,L}} R^{(p)}_{m\,k}(\rho)\,e^{ikz}e^{im\varphi}, \;\; p = 0,1,2,3 \tag{4}$$

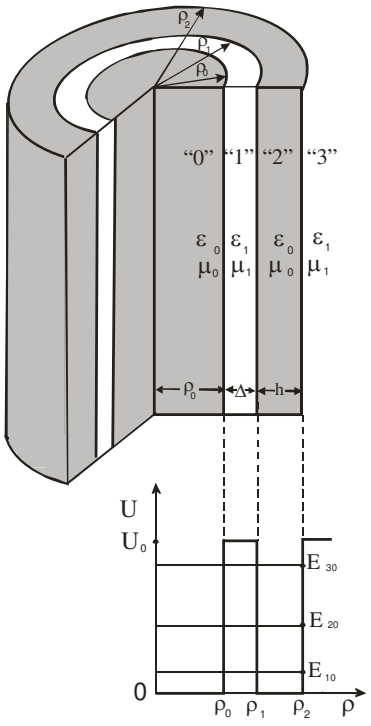

Fig. 1. Geometrical and energy diagrams of a combined cylindrical nanotube

with the radial functions

$$R^{(p)}_{mk}(\rho) =$$

$$= \begin{cases} A^{(0)}_m J_m(\chi_0\rho), & 0 \le \rho \le \rho_0, \\ A^{(1)}_m I_m(\chi_1\rho) + B^{(1)}_m K_m(\chi_1\rho), & \rho_0 \le \rho \le \rho_1, \\ A^{(2)}_m J_m(\chi_0\rho) + B^{(2)}_m N_m(\chi_0\rho), & \rho_1 \le \rho \le \rho_2, \\ B^{(3)}_m K_m(\chi_1\rho), & \rho \ge \rho_2. \end{cases} \tag{5}$$

Here,

$$\chi_0 = \sqrt{2\mu_0 E/\hbar^2 - k^2}, \quad \chi_1 = \sqrt{2\mu_1(U_0 - E)/\hbar^2 + k^2}, \tag{6}$$

k is the axial quasimomentum; $m = 0, \pm1, \pm2, \ldots$ is the magnetic quantum number; L is the size of the effective region for the electron motion along the nanotube axis; J_m and N_m are the Bessel and Neumann, respectively, functions of integer order; and I_m and K_m are the modified Bessel and Macdonald, respectively, functions [15].

Conditions for the wave functions and the corresponding density probability flows to be continuous across all

the three interfaces in the nanosystem (at $\rho = \rho_0$, ρ_1, and ρ_2),

$$\begin{cases} R^{(p)}_{m\,k}(\rho_p) = R^{(p+1)}_{m\,k}(\rho_p), \quad (p = 0, 1, 2) \\ \dfrac{1}{\mu_p}\dfrac{\partial R^{(p)}_{m\,k}(\rho)}{\partial \rho}\Big|_{\rho=\rho_p} = \dfrac{1}{\mu_{p+1}}\dfrac{\partial R^{(p+1)}_{m\,k}(\rho)}{\partial \rho}\Big|_{\rho=\rho_p}, \end{cases} \tag{7}$$

together with the normalization condition

$$\int\limits_0^\infty |R_{m\,k}(\rho)|^2\, \rho d\rho = 1 \tag{8}$$

allow us to determine all unknown coefficients $A^{(p)}_m$ and $B^{(p)}_m$ $(p = 0, 1, 2, 3)$ in Eq. ([5]) and, therefore, to obtain the analytical expressions for the wave functions $\psi_{n_\rho mk}(\mathbf{r})$ and the dispersion equation. The solutions of the latter are enumerated by the radial quantum number $n_\rho = 1, 2, \ldots$ and determine the electron energy spectrum $E_{n_\rho m}(k)$.

3. Interaction of an Electron with Confined and Interface Phonons in a Combined Cylindrical Nanotube

In the dielectric continuum model, the polarization field of a combined nanotube is described by the system of Maxwell equations for the corresponding media,

$$\begin{cases} \mathbf{D} = \varepsilon(\rho, \omega)\,\mathbf{E} = \mathbf{E} + 4\pi\mathbf{P}, \\ \mathbf{E} = -\nabla\Phi, \\ \nabla\mathbf{D} = 0, \end{cases} \tag{9}$$

where $\mathbf{D}$ is the vector of electric field induction, Φ the polarization field potential, and $\mathbf{P}$ the polarization vector. From system (9), we obtain the equation

$$\boldsymbol{\nabla}\left(\varepsilon(\rho, \omega)\ \boldsymbol{\nabla}\Phi(\mathbf{r})\right) = 0, \tag{10}$$

which has two probable solutions. This circumstance is connected with the existence of phonon fields of the following two types [16, 17]:
a) the polarization field of confined phonons, which corresponds to the conditions

$$\varepsilon_p(\rho, \omega) = 0, \quad \Delta\Phi_{L_p}(\mathbf{r}) \neq 0, \quad p = 0, 1, 2, 3, \tag{11}$$

b) and the polarization field of interface phonons, which corresponds to the conditions

$$\varepsilon_p(\rho, \omega) \neq 0, \quad \Delta\Phi_{I_p}(\mathbf{r}) = 0, \quad p = 0, 1, 2, 3. \tag{12}$$

Below, we describe how the energy spectra for all phonon branches and the corresponding potentials in the nanotube can be obtained.

3.1. Confined Phonons

The dielectric permittivity of each semiconductor layer in the combined nanotube is assumed to be a known function of the frequency

$$\varepsilon_p(\omega) = \varepsilon_{p\infty}\frac{\omega^2 - \omega^2_{L_p}}{\omega^2 - \omega^2_{T_p}}, \quad p = 0, 1, \tag{13}$$

where $\varepsilon_{p\infty}$ is the high-frequency dielectric permittivity, and ω_{Lp} and ω_{Tp} are the frequencies of longitudinal and transverse, respectively, phonons in the corresponding massive crystal. From Eqs. (11) and (13), one can see that the spectrum of characteristic energies for confined phonons in the cylindrical nanotube coincides with the frequencies of longitudinal optical phonons in the corresponding massive crystals that the nanotube is made up of,

$$\Omega_{L_p} = \hbar\omega_{L_p}. \tag{14}$$

Afterward, we find the polarization field potential $\Phi_L(\mathbf{r})$ and the corresponding component of the displacement vector $\mathbf{u}_L$, which are induced by confined optical phonons. For this purpose, taking the cylindrical symmetry of the system into consideration, the components of the potential $\Phi_L(\mathbf{r})$ in every nanosystem region are tried in the form of a series expansion in a complete set of cylindrically symmetric functions

$$\Phi_{L_0}(\mathbf{r})\,|_{\rho\leq\rho_0} = \sum_{mk_0q} \Phi_{mq}(k_0) B_{k_0} J_m(k_0\rho) e^{iqz} e^{im\varphi},$$

$$\Phi_{L_p}(\mathbf{r})\,|_{\rho_{p-1}\leq\rho\leq\rho_p} =$$

$$= \sum_{mk_pq} \Phi_{mq}(k_p)\left(B_{k_p} J_m(k_p\rho) + A_{k_p} N_m(k_p\rho)\right) e^{iqz} e^{im\varphi},$$

$$(p = 1, 2),$$

$$\Phi_{L_3}(\mathbf{r})\,|_{\rho\geq\rho_2} = \sum_{mk_3q} \Phi_{mq}(k_3) A_{k_3} N_m(k_3\rho) e^{iqz} e^{im\varphi}. \tag{15}$$

Here, $J_m(k_p\rho)$ and $N_m(k_p\rho)$ are the Bessel and Neumann, respectively, functions of integer order, and q is the axial quasimomentum. All unknown coefficients A_{k_p}, B_{k_p}, and $\Phi_{mq}(k_p)$, as well as the quasiwave numbers k_p, are determined from the conditions for the polarization potentials to be zero at the interfaces between nanosystem media and the orthonormality condition for the complete set of functions used at quantizing this

phonon field. As a result, we obtain the Hamiltonian of interaction between the electron and the polarization field $\widehat{\Phi}_L(\mathbf{r})$ in the secondary quantization representation for phonon variables and the coordinate representation for electron ones,

$$\hat{H}_{e-L}\,(\rho,\varphi,z) = -e\,\hat{\Phi}_L(\mathbf{r}) =$$

$$= -\sqrt{\frac{2e^2\Omega_{L_0}}{L}\left(\frac{1}{\varepsilon_{\infty 0}}-\frac{1}{\varepsilon_{00}}\right)}\sum_{m\,q}\frac{1}{\rho_0\sqrt{k_0^2+q^2}}\times$$

$$\times\frac{J_m(k_0\rho)e^{iqz}e^{im\varphi}}{|J_{m+1}(k_0\,\rho_0)|}\,(\hat{b}_{mqk_0}+\hat{b}^{+}_{-m,-q\,k_0})\Big|_{\rho\le\rho_0} -$$

$$-\sum_{p=1}^{2}\sqrt{\frac{2e^2\Omega_{L_p}}{L}\left(\frac{1}{\varepsilon_{\infty p}}-\frac{1}{\varepsilon_{0p}}\right)}\frac{\pi}{2}\sum_{m\,q}\frac{k_p}{\sqrt{k_p^2+q^2}}\times$$

$$\times\left[\frac{1}{N_m^2(k_p\,\rho_p)}-\frac{1}{N_m^2(k_p\,\rho_{p-1})}\right]^{-1/2}\times$$

$$\times\left[J_m\,(k_p\,\rho)-\frac{J_m(k_p\,\rho_{p-1})}{N_m(k_p\,\rho_{p-1})}N_m(k_p\,\rho)\right]\times$$

$$\times e^{iqz}e^{im\varphi}(\hat{b}_{m\,q\,k_p}+\hat{b}^{+}_{-m,-q\,k_p})\Big|_{\rho_{p-1}\le\rho\le\rho_p} -$$

$$-\sqrt{\frac{2e^2\Omega_{L_1}}{L}\left(\frac{1}{\varepsilon_{\infty 1}}-\frac{1}{\varepsilon_{01}}\right)}\quad\sum_{m\,q}\frac{1}{\rho_2\sqrt{k_3^2+q^2}}\times$$

$$\times\frac{N_m(k_3\rho)e^{iqz}e^{im\varphi}}{|N_{m+1}(k_3\,\rho_2)|}\quad\left(\hat{b}_{mqk_3}+\hat{b}^{+}_{-m,-q\,k_3}\right)\Big|_{\rho\,\ge\,\rho_2}. \qquad (16)$$

Here, the operators of secondary quantization $\widehat{b}_{mqk_p}$ and $\widehat{b}^{+}_{mqk_p}$ satisfy the bosonic commutation relation

$$[\,\hat{b}_{mqk_p},\hat{b}^{+}_{m'q'k'_p}] = \delta_{mm'}\delta_{k_pk'_p}\delta_{qq'}. \qquad (17)$$

3.2. Interface Phonons

The polarization field of interface phonons is described by Eqs. (12). Taking the cylindrical symmetry of a nanotube into account, it is expedient to seek the function that would satisfy the Laplace equation in (12) in the form

$$\Phi_I^{(p)}\,(\mathbf{r}) = f_m^{(p)}\,(\rho)\,e^{im\varphi}e^{iqz}\quad(p=0,1,2,3). \qquad (18)$$

The substitution of Eq. (18) into Eq. (12) brings about the Bessel equation for the function $f_m^{(p)}$,

$$\left(\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}-\left(\frac{m^2}{\rho^2}+q^2\right)\right)f_m^{(p)}\,(\rho)=0, \qquad (19)$$

Its solutions in various ρ-regions are the modified Bessel functions

$$f_{mq}^{(p)}(\rho)=\begin{cases}A_0I_m\,(q\rho)\,, & \rho\le\rho_0,\\ A_1I_m\,(q\rho)+B_1K_m\,(q\rho)\,, & \rho_0\le\rho\le\rho_1,\\ A_2I_m\,(q\rho)+B_2K_m\,(q\rho)\,, & \rho_1\le\rho\le\rho_2,\\ B_3K_m\,(q\rho)\,, & \rho\ge\rho_2.\end{cases} \qquad (20)$$

In accordance with electrodynamics laws, the potential of the interface phonon polarization field, Φ_I, must be such that the tangential component of the field strength and the normal component of the induction should be continuous across each interface in the combined cylindrical nanotube,

$$\mathbf{E}_{\tau_p}\,(\rho_p)=\mathbf{E}_{\tau_{p+1}}\,(\rho_p)\,,\quad \mathbf{D}_{n_p}\,(\rho_p)=\mathbf{D}_{n_{p+1}}\rho_p,$$

$$(p=0,1,2). \qquad (21)$$

Boundary conditions (21) lead to a system of linear homogeneous equations for the unknown coefficients A_p and B_p. This system is used to derive the dispersion equation, the solutions of which, $\omega_{ms}(q)$, are enumerated by the quantum number s and determine the energy spectrum of interface phonons in the system,

$$\Omega_{m\,s}(q)=\hbar\,\omega_{m\,s}(q) \qquad (22)$$

as well as the coefficients A_p and B_p. The dispersion equation and the expressions for A_p and B_p are very cumbersome so that their explicit forms are not presented here.

Thus, the Hamiltonian of interaction between an electron and the polarization field $\widehat{\Phi}_I(\mathbf{r})$ expressed in the secondary quantization representation for phonon variables and the coordinate representation for electron ones looks like

$$\hat{H}_{e-I}\,(\rho,\varphi,z) = -e\,\hat{\Phi}_I(\mathbf{r}) =$$

$$= -\sum_{mqs}\Phi_{mqs}(\rho)e^{iqs}e^{im\varphi}(\hat{b}_{mqs}+\hat{b}^{+}_{-m,-qs}) =$$

$$= -\sum_{mqs}\sqrt{\frac{\hbar\,e^2}{Ly_{qs}\omega_{ms}(q)}}\,e^{iqz}e^{im\varphi}\times$$

$$\times[\,A_0\,I_m\,(q\rho)|_{\rho\le\rho_0}+B_3\,K_m\,(q\rho)|_{\rho\ge\,\rho_2}+$$

$$+\sum_{p=1}^{2}\,[A_pI_m\,(q\rho)+B_pK_m\,(q\rho)]|_{\rho_{p-1}\le\rho\le\rho_p}]\times$$

$$\times (\hat{b}_{mqs} + \hat{b}^{+}_{-m,-qs})], \tag{23}$$

where

$$y_{qs} = \frac{1}{2}\left(\frac{(\varepsilon_{00} - \varepsilon_{\infty 0})\,\omega_{T0}^2}{(\omega_{ms}^2(q) - \omega_{T0}^2)^2} \rho_0 f_m^{(0)}(\rho_0)\, \frac{\partial f_m^{(0)}(\rho)}{\partial \rho}\bigg|_{\rho_0} + \right.$$

$$+ \frac{(\varepsilon_{01} - \varepsilon_{\infty 1})\,\omega_{T1}^2}{(\omega_{ms}^2(q) - \omega_{T1}^2)^2} \rho_2 f_m^{(3)}(\rho_2)\, \frac{\partial f_m^{(3)}(\rho)}{\partial \rho}\bigg|_{\rho_2} +$$

$$\left. + \sum_{p=1}^{2} \frac{(\varepsilon_{0p} - \varepsilon_{\infty p})\omega_{Tp}^2}{(\omega_{ms}^2(q) - \omega_{Tp}^2)^2} \rho f_m^{(p)}(\rho)\, \frac{\partial f_m^{(p)}(\rho)}{\partial \rho}\bigg|_{\rho_{p-1}}^{\rho_p} \right). \tag{24}$$

The transition in Hamiltonians (16) and (23) to the occupation number representation for electron variables is carried out, following the general theory, by using the quantized wave functions

$$\hat{\Psi}_{n_\rho\, m\, k}(\mathbf{r}) = \sum_{n_\rho\, m\, k} \hat{\Psi}_{n_\rho\, m\, k}(\mathbf{r}) \hat{a}_{n_\rho\, m\, k},$$

$$\hat{\Psi}^{+}_{n_\rho\, m\, k}(\mathbf{r}) = \sum_{n_\rho\, m\, k} \hat{\Psi}^{*}_{n_\rho\, m\, k}(\mathbf{r}) \hat{a}^{+}_{n_\rho\, m\, k}, \tag{25}$$

where $\widehat{a}_{n_\rho mk}$ and $\widehat{a}^{+}_{n_\rho mk}$ are the Fermi operators of annihilation and creation, respectively, of electron states described by the wave functions $\Psi_{n_\rho m\, k}(\mathbf{r})$ (Eq. (4)). As a result, the Hamiltonian of electrons and the electron–phonon interaction in the secondary quantization representation for all variables looks like

$$\hat{H} = \int \Psi^{+}_{n_\rho mk}(\mathbf{r}) \left(\hat{H}_e(\mathbf{r}) + \hat{H}_{e-L}(\mathbf{r}) + \right.$$

$$\left. + \hat{H}_{e-I}(\mathbf{r})\right) \Psi^{'}_{n_\rho' m' k}(\mathbf{r}) d^3\mathbf{r} =$$

$$= \hat{H}_e + \hat{H}_{e-L} + \hat{H}_{e-I}\ . \tag{26}$$

Here,

$$\hat{H}_e = \sum_{n_\rho mk} E_{n_\rho m}(k)\, \hat{a}^{+}_{n_\rho mk}\, \hat{a}_{n_\rho mk} \tag{27}$$

is the Hamiltonian of electrons in the representation of their occupation numbers,

$$\hat{H}_{e-L} = \sum_{p=0}^{3} \sum_{kqk_p} \sum_{mm_1} \sum_{n_{\rho 1} n_{\rho 2}} F^{n_{\rho 2} m_1+m}_{n_{\rho 1}\, m_1\, k}(m,q,k_p) \times$$

$$\times \hat{a}^{+}_{n_{\rho 1}\, m_1\, k+q}\, \hat{a}_{n_{\rho 2}\, m_1+m\, k} \left(\hat{b}^{+}_{mqk_p} + \hat{b}_{-m-qk_p}\right) \tag{28}$$

is the Hamiltonian of interaction between the electron and confined L-phonons, which contains the coupling functions

$$F^{n_{\rho 2}\, m_1+m}_{n_{\rho 1}\, m_1\, k}(m,q,k_0) =$$

$$= \sqrt{\frac{2\,e^2\,\Omega_{L\,0}}{L}\left(\frac{1}{\varepsilon_{\infty\,0}} - \frac{1}{\varepsilon_{0\,0}}\right)} \frac{1}{\rho_0\sqrt{k_0^2+q^2}} \frac{1}{|J_{m+1}(k_0\rho_0)|} \times$$

$$\times \int_0^{\rho_0} R^{*}_{n_{\rho 1}\, m_1\, k+q}(\rho)\, R_{n_{\rho 2}\, m_1+m\, k}(\rho)\, J_m(k_0\rho)\, \rho\, d\rho, \tag{29}$$

$$F^{n_{\rho 2}\, m_1+m}_{n_{\rho 1}\, m_1\, k}(m,q,k_3) =$$

$$= \sqrt{\frac{2\,e^2\,\Omega_{L\,1}}{L}\left(\frac{1}{\varepsilon_{\infty\,1}} - \frac{1}{\varepsilon_{0\,1}}\right)} \frac{1}{\rho_2\sqrt{k_3^2+q^2}} \frac{1}{|N_{m+1}(k_3\rho_0)|} \times$$

$$\times \int_{\rho_2}^{\infty} R^{*}_{n_{\rho 1}\, m_1\, k+q}(\rho)\, R_{n_{\rho 2}\, m_1+m\, k}(\rho)\, N_m(k_3\rho)\, \rho\, d\rho, \tag{30}$$

$$F^{n_{\rho 2}\, m_1+m}_{n_{\rho 1}\, m_1\, k}(m,q,k_{p=1,2}) =$$

$$= \sqrt{\frac{2\,e^2\,\Omega_{L\,p}}{L}\left(\frac{1}{\varepsilon_{\infty\,p}} - \frac{1}{\varepsilon_{0\,p}}\right)} \frac{\pi}{2} \frac{k_p}{\sqrt{k_p^2+q^2}} \times$$

$$\times \left[\frac{1}{N_m^2(k_p\rho_p)} - \frac{1}{N_m^2(k_p\rho_{p-1})}\right]^{-1/2} \times$$

$$\times \int_{\rho_{p-1}}^{\rho_p} R^{*}_{n_{\rho 1}\, m_1\, k+q}(\rho)\, R_{n_{\rho 2}\, m_1+m\, k}(\rho) \times$$

$$\times \left[J_m(k_p\rho) - \frac{J_m(k_p\rho_{p-1})}{N_m(k_p\rho_{p-1})} N_m(k_p\rho)\right] \rho\, d\rho. \tag{31}$$

and

$$\hat{H}_{e-I} = \sum_{kqs} \sum_{mm_1} \sum_{n_{\rho 1} n_{\rho 2}} F^{n_{\rho 2}\, m_1+m}_{n_{\rho 1}\, m_1\, k}(m,q,s) \times$$

$$\hat{a}^{+}_{n_{\rho 1}\, m_1\, k+q}\, \hat{a}_{n_{\rho 2}\, m_1+m\, k} \left(\hat{b}^{+}_{mqs} + \hat{b}_{-m-qs}\right) \tag{32}$$

is the Hamiltonian of interaction between the electron and interface I-phonons, which contains the coupling functions

$$F^{n_{\rho 2}\, m_1+m}_{n_{\rho 1}\, m_1\, k}(m,q,s) =$$

$$= \sqrt{\frac{e^2\,\Omega_{m\,s}(q)}{L y_{q\,s}}} \int_0^{\infty} R^{*}_{n_{\rho 1}\, m_1\, k+q}(\rho)\, R_{n_{\rho 2}\, m_1+m\, k}(\rho)\, \rho\, d\rho \times$$

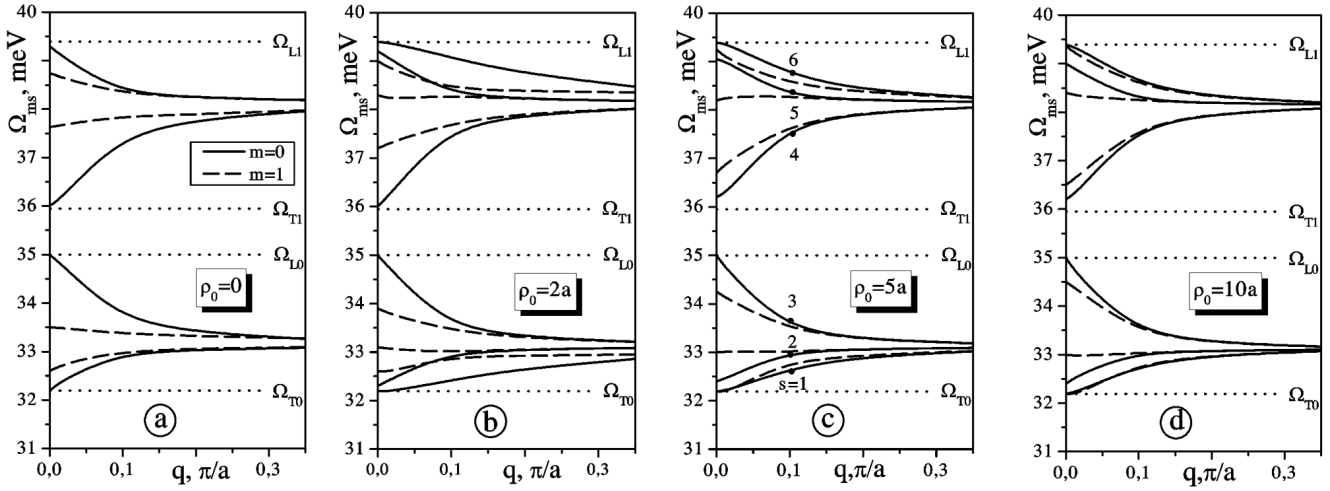

Fig. 2. Dependences of the energy of confined and interface phonons on the axial quasimomentum q at the fixed thicknesses of the nanotube, $h = 7a$, and the layer-barrier, $\Delta = 4a$, and for various radii of the core wire, ρ_0

$$\times[I_m(q\rho)_{\rho\le\rho_0} + B_3\, K_m(q\rho)|_{\rho\ge\rho_2} + \\ + \sum_{p=1}^{2} [A_p I_m(q\rho) + B_p K_m(q\rho)]|_{\rho_{p-1}\le\rho\le\rho_p}\Big]. \quad (33)$$

The obtained Hamiltonian (26) is basic, while analyzing the renormalization of the energy spectrum of electrons by their interaction with confined and interface phonons. Its advantage consists in that the form obtained is suitable for the application of methods of quantum field theory, in particular, the Green's function method and the Feynman's diagram technique. This circumstance allows us to study various versions with all possible coupling forces between quasiparticles and phonons in a combined cylindrical nanotube.

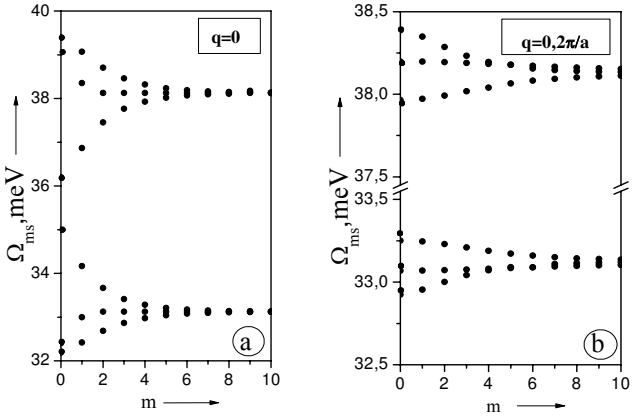

Fig. 3. Dependences of the interface phonon energy Ω_{ms} on m at $\rho_0 = 5a$, $\Delta = 4a$, $h = 7a$ and $q = 0$ (a) or $0.2\pi/a$ (b)

4. Analysis and Discussion of Results

In work [12], we studied the dependences of the electron and exciton spectra on the geometrical parameters of a combined cylindrical semiconductor nanotube in detail. Therefore, now let us analyze the phonon spectra and the polarization field potentials in a cylindrical nanotube made up of GaAs (medium 0) and $Al_{0.4}Ga_{0.6}As$ (medium 1) semiconductors. Their material parameters are as follows: the energy of longitudinal and transverse optical phonons in the corresponding media are $\Omega_{L0} = 35$ meV, $\Omega_{T0} = 32.2$ meV, $\Omega_{L1} = 39.4$ meV, and $\Omega_{T1} = 35.95$ meV; the lattice constants are $a = a_0 \approx a_1 = 5.65$ Å; and the dielectric permittivities are $\varepsilon_{\infty 0} = 10.85$ and $\varepsilon_{\infty 1} = 9.8$.

The results of calculations of the phonon spectrum for the examined nanosystem at fixed thicknesses (typical of experimentally created nanosystems [8]) of a nanotube, $h = 7a$, and a layer-barrier, $\Delta = 4a$, and various radii of a core wire, ρ_0, are depicted in Fig. 2, which illustrates the properties of this spectrum and its evolution with the variation of nanosystem geometrical parameters.

From Fig. 2,a, one can see that, if the internal medium is absent, i.e. $\rho_0 = 0$, the phonon spectrum includes the dispersion-free energies of confined phonons, Ω_{L0} and Ω_{L1}, and four groups with the infinite number of branches ($m = 0, 1, \ldots$) with a weak q-dispersion for the energies of interface phonons, $\Omega_{ms}(q)$. In Fig. 2, only the branch $\Omega_{m=0,1s}(q)$ is shown. The Ω_{ms}-values calculated for other m and $\rho_0 = 5a$ are exhibited in Fig. 3,a (for $q = 0$) and Fig. 3,b (for $q = 0.2\pi/a$).

From Fig. 2,a, it is also evident that, at $m = 0$ and 1, two branches of I-phonons have a positive dispersion,

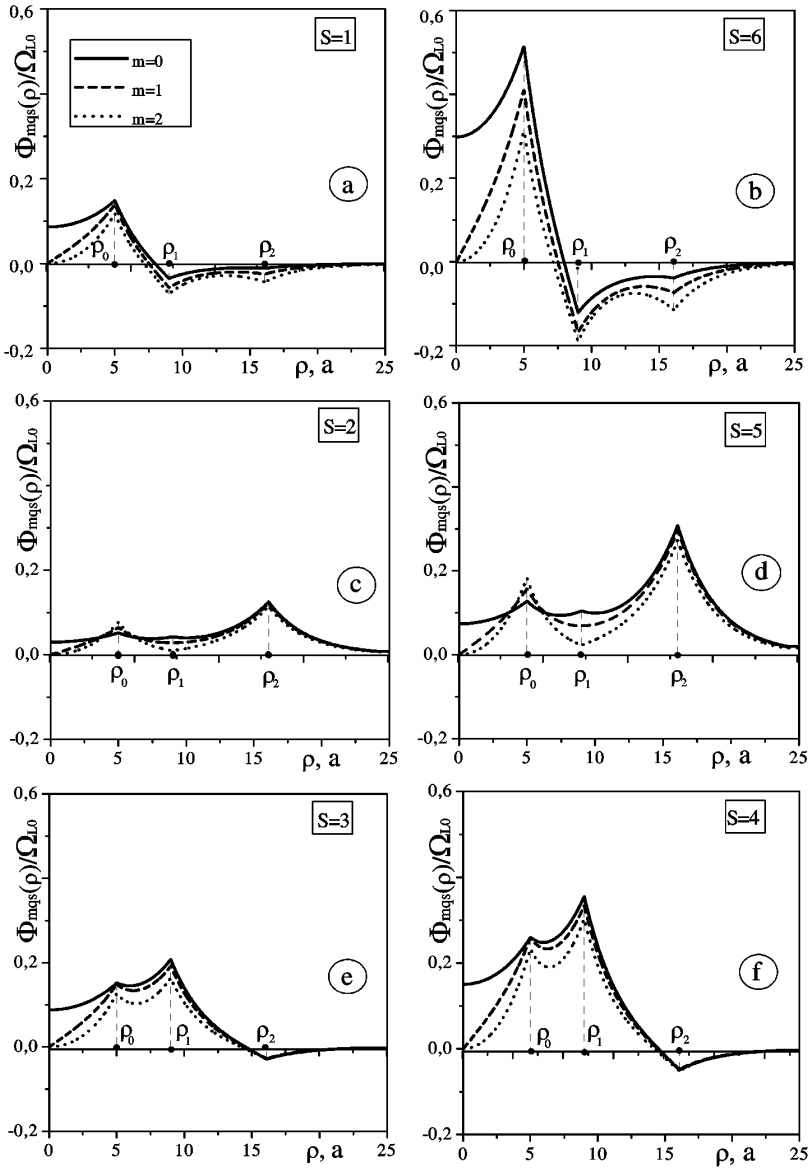

Fig. 4. Dependences of the potential Φ_{mqs} on ρ at $q = 0.2\pi/a$, $\rho_0 = 5a$, $h = 7a$, and $\Delta = 4a$

and two others have a negative one. The energy of every upper I-phonon group lies within the interval between Ω_{L1} and Ω_{T1}, and that of every lower I-phonon group lies between Ω_{L0} and Ω_{T0}.

However, if the cylindrical nanotube has the internal radius $\rho_0 \neq 0$ (Figs. 2,*b* to *d*), two more groups of branches appear in the spectrum of interface phonons: a group with a positive dispersion in the low-energy range, $\Omega_{m2}(q)$, and a group with a negative dispersion in the high-energy one, $\Omega_{m5}(q)$. The physical reason for the presence of four (at $\rho_0 = 0$) or six (at $\rho_0 \neq 0$) groups of branches for interface phonons consists in the existence of two or three, respectively, interfaces GaAs/$Al_{0.4}Ga_{0.6}As$ between semiconductor media (Fig. 1).

From Figs. 2,*b* to *d*, one can see that, if the tube width is fixed, the dispersion of interface phonons is sensitive to the ρ_0-value only at small q's. In the range $q \geq 0.1\pi/a$, the energy of interface phonons practically does not change irrespective of the ρ_0-value.

From Fig. 3, it is evident than the m-dispersion of interface phonons in all groups is also insignificant and is similar to the q-dispersion. This fact is absolutely clear, because it is just the quantum number m that transforms

into the quasimomentum directed perpendicularly to the direction of q in the limit $\rho_0 \to \infty$. It is so, because, in this case, a cylindrical nanotube transforms into a combined plane nano-heterosystem with the geometrical parameters Δ and h.

In Fig. 4, the potential dependences $\Phi_{mqs}(\rho)$ calculated at $q = 0.2\pi/a$, $\rho_0 = 5a$, $h = 7a$, $\Delta = 4a$, and various magnetic quantum numbers $m = 0, 1, 2$ and reckoned in units of Ω_{L0} are depicted for six branches of interface vibrations shown in Fig. 2,*c* and enumerated by the index s. The panels demonstrate that, irrespective of the branch number s, the potential energy of interface phonons nonmonotonously depends on ρ, reaching its extreme values at the interface between semiconductor media that compose the combined nanotube.

Among those six panels, we can distinguish pairs, in which the potential dependence $\Phi_{mqs}(\rho)$ is qualitatively identical within the whole interval of ρ variation. In particular, Fig. 4,*a* corresponds to an interface phonon with the energy Ω_{m1} and the positive q-dispersion, whereas Fig. 4,*b* to an interface phonon with the energy Ω_{m6} and the negative q-dispersion. The maximum potential value for those vibrations is reached at the interface $\rho = \rho_0$. Analogous pairs can be distinguished for potentials with a maximum value at the interface $\rho = \rho_2$ and the corresponding energies Ω_{m2} (positive dispersion) and Ω_{m5} (negative dispersion) – see Figs. 4,*c* and *d* – and for potentials with a maximum value at the interface $\rho = \rho_1$ and the corresponding energies Ω_{m3} (negative dispersion) and Ω_{m4} (positive dispersion) (see Figs. 4,*e* and *f*). The absolute value of potential in every pair at an arbitrary ρ is higher for the component, for which the energy of the corresponding interface phonon Ω_{ms} is larger.

For every s-th branch ($s = 1 \div 6$), the potential of interface phonons at $m = 0$ differs from zero even at $\rho = 0$. However, for all other m, $\Phi_{m\neq 0qs}(\rho = 0) = 0$.

At last, we note that the potential of interface phonon field is maximum at heterointerfaces and quickly falls down as the distance from the interface between semiconductor media increases. Therefore, the renormalization of the electron spectrum by those phonons should be considerable only in superthin nanotubes, in which the maximum of the squared absolute value of electron wave function is also localized near the interface.

5. Conclusions

A theory of the electron–phonon interaction in a combined cylindrical semiconductor nanotube has been developed in the framework of the effective mass model for electrons and a dielectric continuum one for phonons. Analytical expressions are derived for the Hamiltonians of interaction between the electron and confined and interface phonons in the secondary quantization representation for electron and phonon variables. It is found that, in the combined nanotube, there are two dispersion-free branches for confined phonons and six branches for interface ones with weak dispersions with respect to both the magnetic quantum number m and the axial quasimomentum q. Provided that the tube width is fixed, the dispersion of interface phonons is sensitive to variations of the core wire radius ρ_0 only at small q's. The potential of interface phonons is shown to depend nonmonotonously on ρ, irrespective of the phonon spectrum branch, and reach its extreme values at the interfaces between semiconductor media that the combined nanotube is composed of.

The authors are sincerely grateful to Doctor of Phys.-Math. Sci. Prof. M.V. Tkach for the discussion of the results obtained and for his useful advice in the course of preparation of this paper.

1. K. Suenaga, C. Colliex, N. Demoncy, A. Loiseau, H. Pascard, and F. Willaime, Science **278**, 653 (1997).
2. Y. Zhang, K. Suenaga, C. Colliex, and S. Iijima, Science **281**, 973 (1998).
3. A.I. Persson, M.W. Larsson, S. Stenstro, B.J. Ohlsson, L. Samuelson, and L.R. Wallenberg, Nature Mater. **3**, 677 (2004).
4. V.G. Dubrovskii, G.E. Tsyrlin, and V.M. Ustinov, Fiz. Tekh. Poluprovodn. **43**, 1585 (2009).
5. P. Mohan, J. Motohisa, and T. Fukui, J. Phys. Condens.Matter **88**, 013110 (2006).
6. P. Mohan, J. Motohisa, and T. Fukui, Appl. Phys. Lett. **88**, 133105 (2006).
7. M. Heigoldt, J. Arbiol, D. Spirkoska, J.M. Rebled, C.S. Conesa-Boj, G. Abstreiter, F. Peiro, J.R. Morantece, and A. Fontcuberta i Morral, J. Mater. Chem. **19**, 840 (2009).
8. A. Fontcuberta i Morral, D. Spirkoska, J. Arbiol, M. Heigoldt, J.R. Morante, and G. Abstreiter, Small **4**, 899 (2008).
9. X.F. Wang and X.L. Lei, Phys. Rev. B **49**, 4780 (1994).
10. N. Tkach, A. Makhanets, and N. Dovganiuk, Phys. Solid State **51**, 2529 (2009).
11. M. Tkach, O. Makhanets, M. Dovganiuk, and O. Voitsekhivska, Physica E **41**, 1469 (2009).
12. O. Makhanets, N. Tsiupak, and O. Voitsekhivska, in *Proceedings of the 12th International Balkan Workshop on Applied Physics*, edited by V. Ciupina, H. Alexandru,

and M. Cirty (Ovidius Univ. Press, Constanta, 2011), p. 94.

13. S.I. Pekar, *Research in Electron Theory of Crystals* (United States Atomic Energy Commission, Washington, DC, 1963).
14. L.D. Landau and S.I. Pekar, Zh. Èksp. Teor. Fiz. **18**, 419 (1948); L.D. Landau and S.I. Pekar, Ukr. J. Phys. **53**, Special issue, 71 (2008).
15. E. Jahnke, F. Emde, and F. Lösch, *Tafeln höherer Funktionen* (Teubner, Stuttgart, 1960).
16. M.A. Stroscio and M. Dutta, *Phonons in Nanostructures* (Cambridge Univ. Press, Cambridge, 2001).
17. M. Tkach, *Quasiparticles in Nanoheterosystems* (Ruta, Chernivtsi, 2003) (in Ukrainian).

Received 29.11.11.
Translated from Ukrainian by O.I. Voitenko

ФОНОННІ СПЕКТРИ ТА ЕЛЕКТРОН-ФОНОННА ВЗАЄМОДІЯ У СКЛАДНІЙ ЦИЛІНДРИЧНІЙ НАПІВПРОВІДНИКОВІЙ НАНОТРУБЦІ

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Р е з ю м е

У моделі ефективних мас для електрона та діелектричного континууму для фононів розвинуто теорію електрон-фононної взаємодії у складній циліндричній напівпровідниковій нанотрубці. Одержано аналітичні вирази для гамільтоніанів взаємодії електрона з обмеженими та інтерфейсними фононами у зображенні вторинного квантування за електронними і фононними змінними. Досліджено залежності фононних енергій та потенціалу поля поляризації інтерфейсних фононів від аксіального квазіімпульсу та геометричних параметрів складної нанотрубки на основі напівпровідників GaAs та $Al_{0,4}Ga_{0,6}As$.