Digest Journal of Nanomaterials and Biostructures Vol. 6, No 1, January-March 2011, p. 331-339

ELECTRON-OPTICAL PHONON INTERACTION IN CORE-SHELL NANOCOLUMN HETEROSTRUCTURES MADE OF WURTZITE-TYPE MATERIALS

L. ION, G.A. NEMNES, C. VISAN[a], D.E.N. BRÂNCUS, S. ANTOHE
University of Bucharest, Faculty of Physics, "Materials and devices for electronics and optoelectronics" Research Center, str. Atomistilor, nr. 405, Măgurele-Ilfov, 077125, Romania
[a]Permanent address: "Horia Hulubei" National Institute of Physics and Nuclear Engineering, Department of Elementary particles and Informational Technologies, str. Atomiştilor, nr. 407, Măgurele-Ilfov, 077125, Romania

Fröhlich electron-phonon interaction terms are derived, in the frame of dielectric continuum model, for a core-shell nanocolumn cylindrical heterostructure made of anisotropic uniaxial semiconductors, with optical axis along the heterostructure axis. The electron-phonon coupling functions were obtained in an analytical closed form, which allowed us to consider the polaron problem in such type of heterostructures. Numerical results, for a wurtzite GaN/AlN heterostructure, are presented.

(Received January 24, 2010; accepted January 26, 2011)

Keywords: Phonon, Core-shell; Heterostructure; wurtzite; GaN/AlN

1. Introduction

Understanding the electron-phonon interaction, or Fröhlich interaction, in nanometric structures is of great importance, particularly in the case of III-nitride semiconductors, where it is known that electron-optical phonon coupling plays a main role in determining the mobility of free charge carriers. Most of the studies on Fröhlich interaction in nanostructures are based on the dielectric continuum (DC) model [1]. Some features of optical phonon spectra and electron-optical phonon coupling in q-1D wurtzite-type semiconductor systems were described in the frame of DC model [2-4]. The interface phonon modes and their coupling with conduction band electrons in core-shell wurtzite quantum wires were studied in [4]. The full spectrum of optical phonons as well as their interaction with electrons in a quantum wire and a nanotube made of wurtzite semiconductors were investigated in [5] and [6], respectively.

Recently, the successful growth of GaN/AlN core-shell nanowire heterostructure was reported [7]. The aim of this paper is to investigate confinement effects on optical phonons and electron-phonon interaction in such type of core-shell nanowire heterostructures, made of anisotropic uniaxial semiconductors. It is organized as follows: the DC model appropriate for use with the considered system is introduced in section 2 and the full optical phonon is obtained. Then, Fröhlich Hamiltonian is obtained and discussed in section 3. Numerical results carried out in the case of GaN/AlN core-shell nanowire cylindrical heterostructure are presented and discussed.

2. Phonon Hamiltonian

We consider a type I cylindrical core-shell heterostructure having the radii R_1 and R_2 $(R_1 < R_2)$ made of two uniaxial anisotropic polar materials with the optical axis directed along the axis of the heterostructure. We work in the frame of the dielectric continuum (D.C.) model [1], restricting ourselves to the case of polar crystals having the optical phonon field described by a 3D

real vector field. The numerical results presented in this paper are restricted to the case of GaN/AlN heterostructure, but our method allows one to investigate the properties of optical phonons in type I core-shell heterostructures made of wurtzite-type or layered semiconductors.

According to the uniaxial symmetry involved, the equations of the model are written in terms of three vector fields ($\vec{u}(\vec{r},t)$-the optical phonon field, $\vec{P}(\vec{r},t)$-the polarization field and $\vec{E}(\vec{r},t)$-the electric field):

$$\ddot{\vec{u}}_\alpha(\vec{r},t) = \beta_{11}^\alpha \vec{u}_\alpha(\vec{r},t) + \beta_{12}^\alpha \vec{E}_\alpha(\vec{r},t), \tag{1}$$

$$\vec{P}_\alpha(\vec{r},t) = \beta_{12}^\alpha \vec{u}_\alpha(\vec{r},t) + \beta_{22}^\alpha \vec{E}_\alpha(\vec{r},t), \tag{2}$$

where the index α corresponds to a direction that is either parallel $(\alpha = \|)$ or orthogonal $(\alpha = \perp)$ to the optical axis. With the β-coefficients in eqs. (1,2), a diagonal form of the dielectric tensor is obtained [8], with the components:

$$\varepsilon_\alpha(\omega) = \varepsilon_\alpha(\infty)\frac{\left(\omega_{LO}^\alpha\right)^2 - \omega^2}{\left(\omega_{TO}^\alpha\right)^2 - \omega^2}, \tag{3}$$

where, $\varepsilon_\alpha(\infty)$, ω_{TO}^α and ω_{LO}^α are the high frequency dielectric constant of the corresponding material, the transverse phonon mode frequency and the longitudinal phonon mode frequency along the principal direction α, respectively.

In the electrostatic approximation, starting from the eqs. (1) and (2), one can obtain the relation:

$$\sum_{\alpha=II,\perp} g_\alpha(\omega)\vec{u}_\alpha(\vec{r},\omega) = -\nabla\Phi(\vec{r},\omega), \tag{4}$$

where $g_\alpha(\omega) = \left[\left(\omega_{TO}^\alpha\right)^2 - \omega^2\right]\frac{1}{\beta_{12}^\alpha}$. In each distinct domain of the system the electrostatic potential obeys the following equations:

$$\varepsilon_\|^{(1)}\frac{\partial^2\Phi^{(1)}}{\partial x_3^2} + \varepsilon_\perp^{(1)}\left(\frac{\partial^2\Phi^{(1)}}{\partial x_1^2} + \frac{\partial^2\Phi^{(1)}}{\partial x_2^2}\right) = 0 \text{ for } \rho < R_1, \tag{5}$$

$$\varepsilon_\|^{(2)}\frac{\partial^2\Phi^{(2)}}{\partial x_3^2} + \varepsilon_\perp^{(2)}\left(\frac{\partial^2\Phi^{(2)}}{\partial x_1^2} + \frac{\partial^2\Phi^{(2)}}{\partial x_2^2}\right) = 0, \text{ for } R_1 < \rho < R_2, \tag{6}$$

and,

$$\nabla^2\Phi^{(3)} = 0, \text{ for } \rho > R_2, \tag{7}$$

where, we have denoted $\rho = \left(x_1^2 + x_2^2\right)^{1/2}$.

In terms of the cylindrical coordinates (ρ, z, φ) and considering the usual electrostatic boundary conditions at the interfaces, the electrostatic potential in the domains of the heterostructure is given by the expressions:

$$\Phi^{(1)}(\rho,z,\varphi,\omega) = \sum_{m,q} a_{mq}^{(1)} F_{mq}^{(1)}(\lambda^{(1)}\rho) W_{mq}(z,\varphi), \tag{8}$$

$$\Phi^{(2)}(\rho,z,\omega) = \sum_{mq} a_{mq}^{(1)} F_{mq}^{(2)}(\lambda^{(2)}\rho) W_{mq}(z,\varphi), \tag{9}$$

$$\Phi^{(3)}(\rho,z,\varphi) = \sum_{mq} a_{mq}^{(3)} K_m(|q|\rho) W_{mq}(z,\varphi), \tag{10}$$

where $\lambda^{(1,2)} = \dfrac{|q|}{\sqrt{|s^{(1,2)}(\omega)|}}$, $s^{(1,2)}(\omega) = \varepsilon_{\perp}^{(1,2)}(\omega)/\varepsilon_{\parallel}^{(1,2)}(\omega)$, $F_{mq}^{(1)}(z) = I_{|m|}(z)$ if $s^{(1)}(\omega) > 0$

and , respectively, $F_{mq}^{(1)}(z) = J_{|m|}(z)$, if $s^{(1)}(\omega) < 0$,

$$F_{mq}^{(2)}(\lambda^{(2)}\rho,\omega) = \alpha_{mq}(\omega) f_m^{(1)}(\lambda^{(2)}\rho) + \beta_{mq}(\omega) f_m^{(2)}(\lambda^{(2)}\rho),$$

$$\alpha_{mq}(\omega) = -\lambda^{(2)} R_1 \frac{s^{(2)}(\omega)}{|s^{(2)}(\omega)|}\left[F_{mq}^{(1)}(\lambda^{(1)}R_1) f_m^{(2)\prime}(\lambda^{(2)}R_1) - \sqrt{\frac{|s^{(2)}(\omega)|}{|s^{(1)}(\omega)|}} \frac{\varepsilon_{\perp}^{(1)}(\omega)}{\varepsilon_{\perp}^{(2)}(\omega)} F_{mq}^{(1)\prime}(\lambda^{(1)}R_1) f_m^{(2)}(\lambda^{(2)}R_1) \right],$$

$$\beta_{mq}(\omega) = \lambda^{(2)} R_1 \frac{s^{(2)}(\omega)}{|s^{(2)}(\omega)|}\left[F_{mq}^{(1)}(\lambda^{(1)}R_1) f_m^{(1)\prime}(\lambda^{(2)}R_1) - \sqrt{\frac{|s^{(2)}(\omega)|}{|s^{(1)}(\omega)|}} \frac{\varepsilon_{\perp}^{(1)}(\omega)}{\varepsilon_{\perp}^{(2)}(\omega)} F_{mq}^{(1)\prime}(\lambda^{(1)}R_1) f_m^{(1)}(\lambda^{(2)}R_1) \right],$$

$f_m^{(1)}(z) = I_{|m|}(z)$ and $f_m^{(2)}(z) = K_m(z)$, if $s^{(2)}(\omega) > 0$, $f_m^{(1)}(z) = J_{|m|}(z)$ and $f_m^{(2)}(z) = Y_{|m|}(z)$ if $s^{(2)}(\omega) < 0$; in all the above expressions $J_{|m|}(z)$ and $Y_{|m|}(z)$ are Bessel functions of the first and the second kind , while $I_{|m|}(x)$, and $K_m(x)$ are the modified Bessel functions of the first and the second kind, respectively.

By considering periodic boundary conditions along the optical axis of the system we obtain:

$$W_{mq}(z,\varphi) = (2\pi L)^{-1/2} e^{iqz} e^{im\varphi}, \tag{11}$$

q, and m taking the values $q_r = \dfrac{2\pi r}{L}$ with $r = 0,\pm1,\pm2,...$ and $m = 0,\pm1,\pm2,...$, respectively; L is the length of the heterostructure.

Then, the dispersion law for optical phonons of the heterostructure is given by:

$$f_m(q,\omega) = 0, \tag{12}$$

with

$$f_m(q,\omega) = -\frac{\sqrt{|s_2(\omega)|}}{\varepsilon_{\perp}^{(2)}(\omega)} \frac{F_{mq}^{(2)}(\lambda^{(2)}R_2,\omega)}{F_{mq}^{(2)\prime}(\lambda^{(2)}R_2,\omega)} + \frac{K_m(|q|R_2)}{K_m(|q|R_2)}. \tag{13}$$

The Hamiltonian of the free optical phonons of the heterostructure, H_{ph}, is obtained by starting with the following expression [5] for the energy density of the free optical phonons (*j=1,2*):

$$h^{(j)}(\vec{r}) = \sum_{\alpha=II,\perp} \frac{1}{2}\left[\Pi_{\alpha}^{(j)2}(\vec{r}) + \left(\omega_{TO}^{(j)\alpha}\right)^2 u_{\alpha}^{(j)2}(\vec{r}) - \beta_{12}^{(j)\alpha} E_{\alpha}^{(j)}(\vec{r}) u_{\alpha}^{(j)}(\vec{r}) \right], \tag{14}$$

where $\Pi_{\alpha}^{(j)}$ is the α-component of the momentum density canonically conjugated to the corresponding component of the field $\vec{u}^{(j)}$.

In order to obtain the contributions of all types of phonons to H_{ph}, given by:

$$H_{ph} = \int_V dv\, h = \int_{V_1} dv\, h^{(1)} + \int_{V_2} dv\, h^{(2)}, \tag{15}$$

all the fields in eq. (14) will be developed in terms of the eigenvectors of the phonon field, which verify the orthogonality relation [6]:

$$\left[\omega^2-\left(\omega^{'}\right)^2\right]\cdot\left[\int_{V_1} dv\vec{u}^{(1)*}(\vec{r},\omega)\vec{u}^{(1)}(\vec{r},\omega^{'})+\int_{V_2} dv\vec{u}^{(2)*}(\vec{r},\omega)\vec{u}^{(2)}(\vec{r},\omega^{'})\right]=0\text{, i.e.}$$

$$\left[\omega^2-\left(\omega^{'}\right)^2\right]\iint_V dv\vec{u}^{*}(\vec{r},\omega)\vec{u}(\vec{r},\omega^{'})=0\,. \tag{16}$$

One obtains:

$$\vec{u}^{(j)}(\vec{r})=\sum_{mql\mu}\lambda_{mql}^{(\mu)}\left[\vec{u}_{mql}^{(j)(\mu)}(\vec{r})a_{mql}^{(\mu)}+h.c.\right], \tag{17}$$

where, without loss of generality, $\lambda_{mql}^{(\mu)}$ are considered to be real quantities, depending on $|m|$ and $|q|$; $a_{mql}^{(\mu)}$ and $a_{mql}^{(\mu)^+}$ are the annihilation and creation operators for the phonon mode (m,q,l,μ). For fixed *m*, the index *l* labels the distinct solutions of eq. (12), while μ is the character index. Conventionally, we will choose μ = 1 for quasi-transverse modes confined in the core (q-TO1), μ = 2 for quasi-longitudinal modes confined in the core (q-LO1), μ = 3 for quasi-transverse modes confined in the shell (q-TO2), μ = 4 for quasi-longitudinal modes confined in the shell (q-LO2), μ = 5,6 for interface modes, and μ = 7 for surface modes. The operators $a_{mql}^{(\mu)}$ and $a_{mql}^{(\mu)^+}$ obey typical Bose commutation relations:

$$\left[a_{mql}^{(\mu)},a_{m'q'l'}^{(\mu')}\right]=0\,,\ \left[a_{mql}^{(\mu)^+},a_{m'q'l'}^{(\mu')^+}\right]=0\,,\ \left[a_{mql}^{(\mu)},a_{m'q'l'}^{(\mu')^+}\right]=\delta_{mm'}\delta_{ll'}\delta_{qq'}\delta_{\mu\mu'}\,. \tag{18}$$

Considering the equation of motion $\vec{\Pi}^{(j)}=\dot{\vec{u}}^{(j)}$ the following expression is obtained:

$$\vec{\Pi}^{(j)}(\vec{r})=-i\sum_{mql\mu}\lambda_{mql}^{(\mu)}\omega_{ml}^{(\mu)}(q)\left[\vec{u}_{mql}^{(j)(\mu)}(\vec{r})a_{mql}^{(\mu)}-h.c.\right], \tag{19}$$

and, with eqs. (4) and (17):

$$E_{\alpha}^{(j)}(\vec{r})=\sum_{mql\mu}\lambda_{mql}^{(\mu)}\frac{\left(\omega_{TO}^{(j)\alpha}\right)^2-\left[\omega_{ml}^{(\mu)}(q)\right]^2}{\beta_{12}^{(j)\alpha}}\left[\left(\vec{u}_{mql}^{(j)(\mu)}(\vec{r})\right)_{\alpha}a_{mql}^{(\mu)}+h.c.\right],\ \alpha=\|,\perp\,. \tag{20}$$

By collecting the results (17), (19) and (20) in eqs. (14) and (15) and considering (16) with $\vec{u}_{mql}^{(j)(\mu)*}(\vec{r})=\vec{u}_{-m,-q,l}^{(j)(\mu)}(\vec{r})$, and $\lambda_{mql}^{(\mu)}=\left(\frac{\hbar}{2\omega_{ml}^{(\mu)}(q)}\right)^{1/2}$, the following diagonal form is obtained for the free optical phonon Hamiltonian of the heterostructure:

$$H_{ph}=\sum_{mql\mu}\hbar\omega_{ml}^{(\mu)}(q)\left[a_{mql}^{(\mu)^+}a_{mql}^{(\mu)}+1/2\right]. \tag{21}$$

3. Fröhlich Hamiltonian

Next, we derive the Hamiltonian describing the interaction between the conduction electrons and the optical phonon field (Fröhlich interaction). This interaction is written as:

$$H_{e-ph}=-e\Phi(\vec{r})\,. \tag{22}$$

It is induced by both types of polarization charges which contribute to the electrostatic potential, the volume charges, and the interface charges; in eq. (22) e is the electron charge and $\Phi(\vec{r})$ is the electrostatic potential including the above specified contributions.

By taking into account the forms (8-10) for the electrostatic potential, the development (17) of the phonon vector field and the expression of the constant $\lambda_{mql}^{(\mu)}$ indicated above (eq.(20)), the electron-phonon interaction Hamiltonian is obtained in the form:

$$H_{e-ph} = -\sum_{mql\mu} \Gamma_{ml}^{(\mu)}(q) \left[W_{mq}(z,\varphi) F_m \left(\frac{|q|\rho}{\sqrt{\left| s\left(\omega_{ml}^{(\mu)}(q)\right)\right|}} \right) a_{mql}^{(\mu)} + h.c. \right], \tag{23}$$

where the electron-phonon coupling functions are given by,

$$\Gamma_{ml}^{(\mu)}(q) = \frac{\left(\frac{\hbar e^2}{\varepsilon_0 |q| R_2} \right)^{1/2}}{\left| \left[\varepsilon_{II}(\omega)\varepsilon_{\perp}(\omega) \left(F_m' \left(\frac{|q|R_2}{\sqrt{|s(\omega)|}} \right) \right)^2 \frac{\partial f_m(q,\omega)}{\partial \omega} \right]_{\omega=\omega_{mql}^{(\mu)}} \right|^{1/2}}. \tag{24}$$

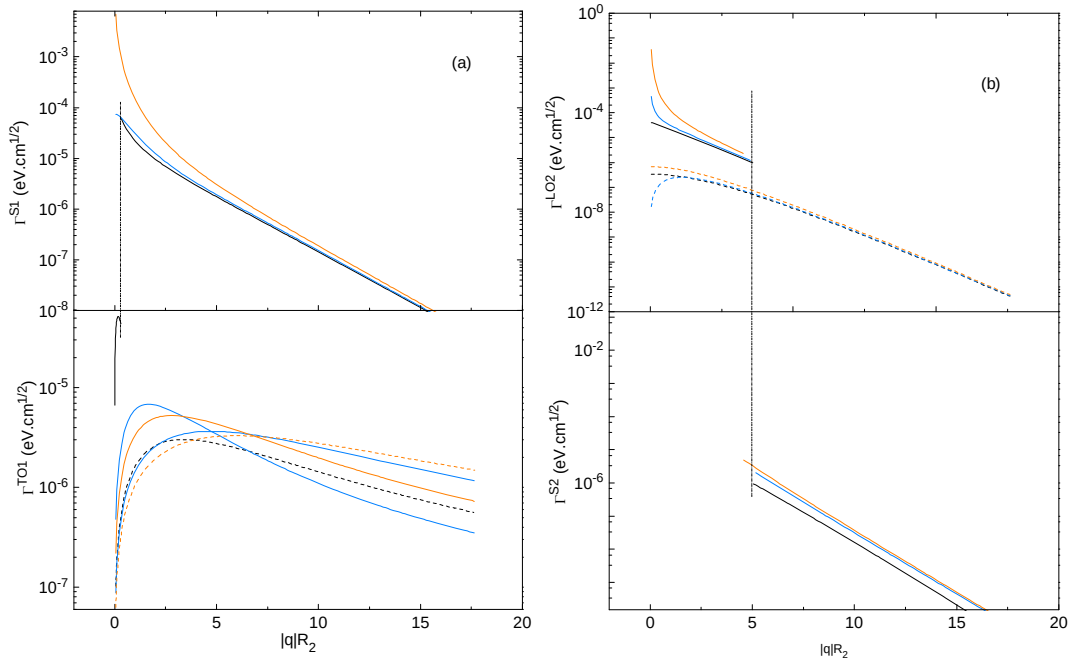

Fig.1. Electron-phonon coupling functions $\Gamma_{ml}^{TO1}(q)$ *and* $\Gamma_{ml}^{S1}(q)$ *(a) and, respectively,* $\Gamma_{ml}^{S2}(q)$ *and* $\Gamma_{ml}^{LO2}(q)$ *(b) for a GaN/AlN cylindrical heterostructure with* R_1/R_2*=0.85. The values of* $|q|R_2$ *where the character is changing from a confined mode to a surface/interface mode are marked with vertical dash-dotted lines. Coupling functions are plotted in black for m=0, in blue for m=1 and orange for m=2. Solid lines correspond to l=1, while dashed lines correspond to l=2.*

Numerical results have been obtained by considering the necessary material parameters for GaN and AlN indicated in [9]. Unlike the case of isotropic semiconductors, the coupling coefficients corresponding to both quasitransverse (q-TO) modes (confined either in the GaN core, or in the AlN barrier of the heterostructure) are not zero (Fig.1a). However, except for q-TO1 mode with *m=0, l=1*, their values are much less than their counterparts for quasilongitudinal or interface/surface modes (Fig.1b). As also seen in the case of a nanowire [5] or nanotube [6] made of anisotropic uniaxial materials, quasitranverse modes with *m=0, l=1* change their character into that of the corresponding surface (in the case of q-TO2) or interface (in the case of q-TO1) mode, irrespective of the R_1/R_2 ratio. In figure 1a the $|q|R_2$ value at which this effect occurs for the q-TO1 mode is marked by the vertical dash-dotted line. The coupling coefficients are continuous across the transition point. The same is true for q-LO2 modes, which change into interface modes (Fig.1b, transition point marked with dash-dotted line). But in this case the position of the transition point and the *m*-value of the q-LO2 mode for which the effect occurs depend on the R_1/R_2 ratio.

3.1 Polaron

In the effective mass approximation, the Hamiltonian of the conduction band electron can be written as *(j=1,2)*:

$$H_e^{(j)} = \frac{p_{\parallel}^{(j)2}}{2m_{\parallel}^{(j)}} + \frac{p_{\perp}^{(j)2}}{2m_{\perp}^{(j)}} + V(\rho), \tag{25}$$

where $p_\alpha^{(j)}$ and $m_\alpha^{(j)}$, $\alpha = \perp, \parallel$, are α-components of electronic momentum and effective mass tensor, respectively. $V(\rho)$ is a confining potential, due to the conduction band offset of the heterostructure ($\Delta E_c = E_c^{(2)} - E_c^{(1)}$):

$$V(\rho) = \begin{cases} 0, & \rho < R_1 \\ \Delta E_c, & R_1 \le \rho < R_2 \\ \infty, & \rho \ge R_2 \end{cases}. \tag{26}$$

The eigenstate of the electron $|kMs\rangle$, with the envelope wave function:

$$\psi_{kMs}(\vec{r}) = \chi_{Ms}(\rho) W_{Mk}(z, \varphi) \tag{27}$$

and the eigen-energy

$$E_{Ms}(k) = \frac{\hbar^2}{2m_{\perp}^{(1)}} \frac{\gamma_{|M|s}^2}{R_1^2} + \frac{\hbar^2 k^2}{2m_{\parallel}^{(1)}} = \Delta E_c - \frac{\hbar^2}{2m_{\perp}^{(2)}} \frac{\xi_{|M|s}^2}{R_1^2} + \frac{\hbar^2 k^2}{2m_{\parallel}^{(2)}} \tag{28}$$

depends on the following quantum numbers: k - the wave number, with values determined by periodic boundary conditions along the optical axis, M - azimuthal quantum number ($M = 0, \pm 1, \pm 2, \ldots$), *s* – radial quantum number, corresponding to *s*-th zero in $\rho = R_2$ of the radial envelope function:

$$\chi_{Ms}(\rho)=C\begin{cases} J_{|M|}\left(\gamma_{|M|s}\dfrac{\rho}{R_1}\right), \rho<R_1 \\ J_{|M|}\left(\gamma_{|M|s}\right)\dfrac{I_{|M|}\left(\xi_{|M|s}\dfrac{\rho}{R_1}\right)K_{Ms}\left(\xi_{|M|s}\dfrac{R_2}{R_1}\right)-I_{|M|}\left(\xi_{|M|s}\dfrac{R_2}{R_1}\right)K_{Ms}\left(\xi_{|M|s}\dfrac{\rho}{R_1}\right)}{I_{|M|}\left(\xi_{|M|s}\right)K_{Ms}\left(\xi_{|M|s}\dfrac{R_2}{R_1}\right)-I_{|M|}\left(\xi_{|M|s}\dfrac{R_2}{R_1}\right)K_{Ms}\left(\xi_{|M|s}\right)}, R_1\le\rho<R_2 \end{cases}$$

The effects of electron-optical phonon interaction are described by the Hamiltonian:

$$H=H_e+H_{ph}+H_{e-ph}. \qquad 29)$$

At $T=0K$, with the electron in the unperturbed state $|k,0,1\rangle$ in the first transverse subband, the total system is in the state $|\Psi_i\rangle=|k,0,1\rangle\otimes|0_{ph}\rangle$, where $|0_{ph}\rangle$ is the vacuum state of the phonon bath; by considering phonon emission processes, we have obtained the free polaron energy in the 2-nd order of Rayleigh-Schrödinger perturbation theory as:

$$E_p(k)=E_{01}(k)-\frac{1}{2\pi L}\sum_{mqls\mu}\frac{\left|G^{(\mu)}_{ml;s}(q)\right|^2}{\hbar\omega^{(\mu)}_{ml}(q)+\dfrac{\hbar^2}{2m^{(1)}_{\|}}(q^2-2kq)+\dfrac{\hbar^2}{2m^{(1)}_{\perp}}\left(\dfrac{\gamma^2_{|M|s}}{R_1^2}-\dfrac{\gamma^2_{01}}{R_1^2}\right)}. \qquad (30)$$

In eq. (30) the following notation was used:

$$\langle\Psi_\nu|H_{e-ph}|\Psi_i\rangle=-\frac{G^{(\mu)}_{ml;s}(q)}{\sqrt{2\pi L}},$$

with the intermediate state $|\Psi_\nu\rangle=|k-q,-m,s\rangle\otimes|1_{ph}(q,m,l)\rangle$. Then, the polaron self-energy E_s and its mass M_p can be obtained, starting from eq. (30), as:

$$E_s=E_p(0)-E_{01}(0) \qquad (31)$$

and, respectively:

$$M_p=\frac{m^{(1)}_{\|}}{1-4\left(\dfrac{2m^{(1)}_{\|}}{\hbar^2}\right)^2\dfrac{1}{2\pi L}\displaystyle\sum_{m,q,l,s,\mu}\frac{q^2\left|G^{(\mu)}_{ml;s}(q)\right|^2}{\left[q^2+\dfrac{m^{(1)}_{\|}}{m^{(1)}_{\perp}}\left(\dfrac{\gamma^2_{|m|s}}{R_1^2}-\dfrac{\gamma^2_{01}}{R_1^2}\right)+\dfrac{2m^{(1)}_{\|}}{\hbar}\omega^{(\mu)}_{ml}(q)\right]^3}}. \qquad (32)$$

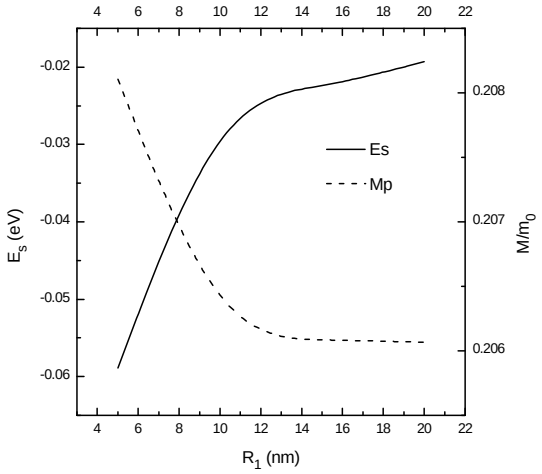

Fig. 2. Self-energy (solid line) and effective mass (dashed line) of the polaron in a GaN/AlN core-shell nanocolumn cylindrical heterostructure as functions on the core GaN radius (R_1/R_2=0.85).

In Fig.2 the values of polaron self-energy and its effective mass as a function of the GaN core radius R_1 are presented; all the phonon branches with m=0,1,2, l=1,2 and the electronic states with M=0,1,2 and s=1,2,3 were included in calculations. The considered R_1/R_2 ratio was 0.85. Both E_s and M_p depends significantly on the core radius for hetersotructures with R_1<12 nm.

4. Conclusions

Using an appropriate form of the energy density of the optical phonon system and the orthogonality relation verified by the eigen-vectors of the optical phonon field, the optical phonon Hamiltonian for a core-shell nanowire cylindrical heterostructure made of uniaxial semiconductors was obtained, as well as the form of the interaction Hamiltonian of optical phonons with a conduction band electron. The electron-phonon coupling functions, for all types of phonons were obtained in an analytical closed form, which allowed to consider the free polaron problem in this type of heterostructure. We found that the contribution of interface/surface phonons is similar in magnitude with that of quasilongitudinal phonon modes and increases with the reduction of the core radius, if the R_1/R_2 ratio is kept constant. As an effect of anisotropy, the electron-quasitransverse phonon modes coupling functions have non-zero values; however, these values are smaller than those corresponding to quasi-longitudinal or interface/surface modes.

Acknowledgements

This work was supported by CNCSIS –UEFISCSU, project number PNII – IDEI 1900/2008.

References

[1] R. Loudon, Adv. Phys. **13**, 423 (1964)
[2] L. Zhang and J.J. Shi, Semicond. Sci. Technol., **20**, 592 (2005)
[3] L. Zhang, J.J. Shi and T.L. Tansley, Phys. Rev. B **71**, 245324 (2005)
[4] L. Zhang and J.J. Shi, Phys. Status Solidi b **243**, 1775 (2006)

[5] D. E. N. Brancus and L. Ion, Phys. Rev. B **76**, 155304 (2007)
[6] D. E. N. Brancus and L. Ion, J. Phys.: Condens. Matter **21**, 485301 (2009)
[7] Hestroffer, R. Mata, D. Camacho, C. Leclere, G. Tourbot, Y. M. Niquet, A. Cros, C. Bougerol, H. Renevier, B. Daudin, Nanotechnology, **21**, 415702 (2010)
[8] D. E. N. Brancus and E. R. Racec, Rom. J. Phys. **45**, 99 (2000)
[9] H. Harima, J. Phys.: Condens. Matter **14**, R967 (2002)