
ELECTRON-PHONON INTERACTION AND THE MECHANISMS OF ELECTRON SPECTRUM RENORMALIZATION IN A FLAT NANOFILM

M.V. TKACH, V.M. KRAMAR

UDC 538.975; 538.915
©2008

Yu. Fed'kovych Chernivtsi National University
(2, Kotsyubynskiy Str., Chernivtsi 58012, Ukraine; e-mail: kramar@itf.cv.ua)

In the framework of the models of dielectric continuum (for phonons) and square potentials and effective masses (for electrons), an expression for the Hamiltonian of electron-phonon interaction, which describes a system consisting of a flat semiconducting film (a quantum well) in a semiconducting medium, has been obtained, where all the system parameters included are given in the occupation-number representation. The Green's function method was applied to analytically calculate the bottom energy of the main electron energy band renormalized by the electron-phonon interaction. Numerical calculations of the shift of the band bottom at the temperature $T = 0$ K were performed, making use of a flat β -HgS/ β -CdS nanoheterosystem as an example. In the case of thin films, the shift has been demonstrated to be governed by the interaction between electrons of the main conduction band and a symmetric mode of interface phonons. In the case of thick nanofilms, the interaction between spatially confined phonons and the electrons from all bands belonging to the discrete part of the system energy spectrum dominates.

1. Introduction

Fundamental and applied researches of nanoheterosystems have been at the center of physicists' attention for a long time [1]. However, although the spectra of quasiparticles – such as electrons, holes, excitons, and phonons – which govern various phenomena in quantum-sized systems, have been studied well enough, the theory of their interaction with quantized and classical fields still remains far from completion.

The overwhelming majority of theoretical works dealing with the electron-phonon and exciton-phonon interactions in quantum wells [2–5], wires [6–8], and dots [9–11] was carried out in the framework of the dielectric continuum model for the phonon subsystem and the models of rectangular potentials and effective masses for electrons, holes, or excitons. The renormalization of the energy spectrum of electrons due to their interaction with phonons in a flat nanofilm was studied either by the method of perturbation theory [3, 5] or by the Lee–Low–Pines variational method [12]. Nanosystems with weak electron-phonon coupling and

at the temperature $T = 0$ K were mainly considered. The Hamiltonian of the system was written down in the occupation-number representation for phonon-related variables and in the coordinate representation for electron-related ones. The methods applied allowed the renormalization of the ground-state-energy values and the effective masses of an electron and a hole, which occurs due to the electron-phonon interaction, to be studied.

However, in the framework of the indicated approaches, systems with intermediate and, all the more, strong electron-phonon coupling cannot be studied. These methods are also inapplicable to the calculation of electron-phonon and exciton-phonon recurrences in nanosystems, although experimental studies of the Raman scattering phenomenon in them are in progress [13]. Hence, there is an urgent need in the development of a consistent theory of electron-phonon and exciton-phonon interaction, which would explain various phenomena occurring in low-dimensional nanostructures with arbitrarily strong coupling and in a wide energy range.

This work was aimed at two goals. The first was to derive a Hamiltonian for the electron-phonon system in a semiconducting nanofilm in the occupation-number representation for all system variables. The solution of this task would enable – in the future – the entire complex of problems belonging to the electron-phonon and exciton-phonon interaction theory to be solved on the basis of the universal Green's function method. The second purpose was to study all mechanisms of interaction between electrons of the main conduction band and all possible phonon branches, which give rise to the renormalization of the main band energy. To this end, we used, as an example, a flat nanofilm created on the basis of the β -HgS/ β -CdS structure [14]. Earlier, such a film was studied theoretically as either a zero-dimensional quantum dot [8] or a one-dimensional quantum wire [9, 10].

It turned out that the results obtained in the framework of such an approach qualitatively correlate – in relevant cases – with the results of calculations executed for similar systems by other methods. So, besides elucidating the role of various mechanisms of electron-phonon interaction and their contribution to the renormalization of the electron spectrum, a reliable basis has been created for the application of the Green's function formalism to the solution of the whole complex of problems in the theory of the interaction between quasiparticles and phonons in nanofilms.

2. Hamiltonian of the Electron-Phonon System in a Nanofilm (a Flat Quantum Well)

2.1. Energy spectrum and wave functions of electron in a flat nanofilm

Consider an electron in a flat semiconducting nanofilm (a quantum well) with the thickness a , which is embedded into a massive external semiconducting medium. The Cartesian coordinate system is so selected that its origin coincides with the film mid-point, and the plane XOY is parallel to the film surface (Fig. 1,*a*). In what follows, nanosystems with small differences between the lattice constants and dielectric permittivities of their components are studied; therefore, the interaction forces between the electron and its electrostatic images [15] are neglected, and the approximations of effective mass and rectangular finite-height potential barriers are used. Hence, the effective mass $m(z)$ and the potential energy $V(z)$ of the electron are considered known (Figs. 1,*b* and *c*):

$$m_{\perp} = \begin{cases} m_0, & V(z) = \begin{cases} 0, & |z| \leq \frac{a}{2}; \\ V, & |z| > \frac{a}{2}. \end{cases} \end{cases} \quad (1)$$

The solution of a stationary Schrödinger equation with the electron Hamiltonian

$$\hat{H}_e = -\frac{\hbar^2 \nabla_{\vec{\rho}}^2}{2m_0} - \frac{\hbar^2}{2} \frac{\partial}{\partial z} \frac{1}{m_{\perp}(z)} \frac{\partial}{\partial z} + V(z) \quad (\vec{\rho} = x\vec{n}_x + y\vec{n}_y), \quad (2)$$

where $\vec{\rho} = x\vec{n}_x + y\vec{n}_y$, is known [5,6]. In the energy range $E_n < V$, the spectrum is determined by the relation

$$E_n(\vec{k}_{\parallel}) = E_n + \frac{\hbar^2 k_{\parallel}^2}{2m_0}, \quad (3)$$

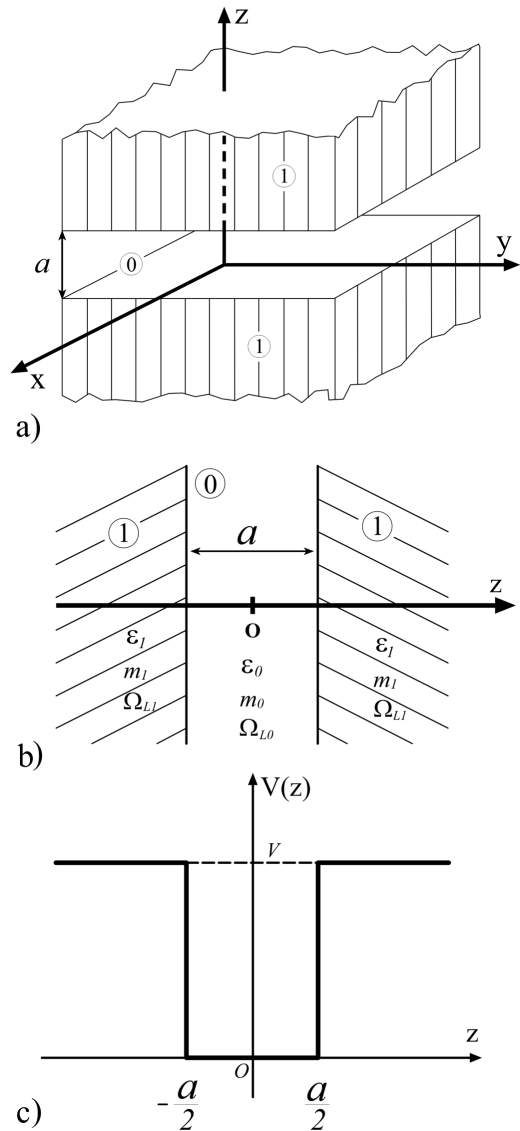


Fig. 1. Geometric models (*a* and *b*) and energy scheme (*c*) of the nanosystem concerned

where $\vec{k}_{\parallel} = k_x\vec{n}_x + k_y\vec{n}_y$, and the E_n -values can be found from the equation

$$\left\{ \operatorname{tg} \left(\frac{a \sqrt{2m_0 E_n}}{\hbar} \right) \right\}^{\pm 1} = \pm \sqrt{\frac{m_0(V - E_n)}{m_1 E_n}}, \quad (4)$$

where the sign + corresponds to odd and the sign – to even n -values. The wave functions of the symmetric

(odd n) and antisymmetric (even n) electron states,

$$\Psi_{n\vec{k}_{\parallel}}(\vec{\rho}, z) = \frac{C_n}{\sqrt{a}} e^{i\vec{k}_{\parallel}\vec{\rho}} \begin{cases} \text{cs}(k_{0n}z), & |z| \leq \frac{a}{2}; \\ \text{cs}[\text{sign}(z)k_{0n}\frac{a}{2}] \times \\ \times \exp([k_{1n}(\frac{a}{2} - |z|)]), & |z| > \frac{a}{2} \end{cases} \quad (5)$$

contain normalizing factors

$$C_n = \sqrt{\frac{2}{1 + (-1)^n \frac{\sin(k_{0n}a)}{k_{0n}a} + 2 \frac{\text{cs}^2(k_{0n}/2)}{k_{0n}a}}} \quad (6)$$

and the transverse components of quasimomenta

$$k_{0n} = \sqrt{2m_0 E_n}/\hbar, k_{1n} = \sqrt{2m_1(V - E_n)}/\hbar, \quad (7)$$

where

$$\text{cs}(x_n) = \begin{cases} \cos x_n, \\ \sin x_n, \end{cases} \quad \text{sc}(x_n) = \begin{cases} \sin x_n, & n = 1, 3, \dots \\ \cos x_n, & n = 2, 4, \dots \end{cases} \quad (8)$$

are the convenient notation introduced for the cumbersome mathematical expressions to be written down in a compact form.

The continuous range of the electron spectrum ($E > V$) is characterized by the dispersion law

$$E(\vec{k}_{\parallel}, k_{\perp}) = V + \frac{\hbar^2}{2m_0}(k_{\parallel}^2 + k_{\perp}^2), \quad (9)$$

and by the following wave functions of an electron: in the symmetric,

$$\Psi_{k_{\perp}\vec{k}_{\parallel}}^{(+)}(\vec{\rho}, z) = \frac{C^+}{\sqrt{L}} e^{i\vec{k}_{\parallel}\vec{\rho}} \times$$

$$\begin{cases} \cos(k_{0\perp}z), & |z| \leq \frac{a}{2}; \\ \cos \frac{k_{0n}a}{2} \cos[k_{1\perp}(|z| - \frac{a}{2})] - \\ \times \sqrt{\frac{m_1 E}{m_0(E - V)}} \times \\ \times \sin \frac{k_{0n}a}{2} \sin[k_{1\perp}(|z| - \frac{a}{2})], & |z| > \frac{a}{2} \end{cases} \quad (10)$$

and antisymmetric,

$$\Psi_{k_{\perp}\vec{k}_{\parallel}}^{(-)}(\vec{\rho}, z) = \frac{C^-}{\sqrt{L}} e^{i\vec{k}_{\parallel}\vec{\rho}} \times$$

$$\begin{cases} \sin(k_{0\perp}z), & |z| \leq \frac{a}{2}; \\ \text{sign}(z) \left(\sin \frac{k_{0n}a}{2} \times \right. \\ \times \cos[k_{1\perp}(|z| - \frac{a}{2})] + \sqrt{\frac{m_1 E}{m_0(E - V)}} \times \\ \left. \times \cos \frac{k_{0n}a}{2} \sin[k_{1\perp}(|z| - \frac{a}{2})] \right), & |z| > \frac{a}{2} \end{cases} \quad (11)$$

states with the corresponding normalizing factors

$$C^{\pm} = \sqrt{\frac{2}{\text{cs}^2(k_{0\perp}a/2) + \frac{m_1 E}{m_0(E - V)} \text{sc}^2(k_{0\perp}a/2)}}, \quad (12)$$

where

$$k_{0\perp} = \sqrt{2m_0 E}/\hbar, k_{1\perp} = \sqrt{2m_1(E - V)}/\hbar. \quad (13)$$

Making a transition to the occupation-number representation for the electron-related variables in Hamiltonian (2) with the help of the quantized wave functions

$$\hat{\Psi}(\vec{\rho}, z) = \sum_{\vec{k}_{\parallel}} \left[\sum_n \hat{a}_{n\vec{k}_{\parallel}} \psi_{n\vec{k}_{\parallel}}(\vec{\rho}, z) + \sum_{k_{\perp}} \hat{a}_{k_{\perp}\vec{k}_{\parallel}} \psi_{k_{\perp}\vec{k}_{\parallel}}(\vec{\rho}, z) \right], \quad (14)$$

we obtain the free-electron Hamiltonian in the secondary quantization representation:

$$\hat{H}_e = \sum_{\vec{k}_{\parallel}} \left[\sum_n E_n(\vec{k}_{\parallel}) \hat{a}_{n\vec{k}_{\parallel}}^+ \hat{a}_{n\vec{k}_{\parallel}} + \sum_{k_{\perp}} E(\vec{k}_{\parallel}, k_{\perp}) \hat{a}_{k_{\perp}\vec{k}_{\parallel}}^+ \hat{a}_{k_{\perp}\vec{k}_{\parallel}} \right], \quad (15)$$

where $\hat{a}_{n\vec{k}_{\parallel}}^+$, $\hat{a}_{n\vec{k}_{\parallel}}$, $\hat{a}_{k_{\perp}\vec{k}_{\parallel}}^+$, and $\hat{a}_{k_{\perp}\vec{k}_{\parallel}}$ are the creation and annihilation operators for the corresponding electron states.

2.2. Hamiltonian of confined, semiconfined, and interface phonons

The Hamiltonian and the polarization potential of free phonons in our nanosystem are obtained in the framework of the dielectric continuum model, where, according to the general theory [16], the dielectric permittivities of both media ($l = 0$ or 1)

$$\varepsilon_l(\omega) = \omega_{\infty}^{(l)} \frac{\hbar^2 \omega^2 - \Omega_{Ll}^2}{\hbar^2 \omega^2 - \Omega_{Tl}^2} \quad (16)$$

are considered known and described by the Lyddane–Sachs–Teller functions.

Quantization of the phonon field was carried out in work [5]. In terms of the compact convenient notations, the Hamiltonian of free phonons can be written down as follows:

$$\begin{aligned} \hat{H}_{\text{ph}} &= \hat{H}_{L0} + \hat{H}_{L1} + \hat{H}_I = \sum_{\lambda, \vec{q}_{\parallel}} \Omega_{L0} (\hat{b}_{\lambda \vec{q}_{\parallel}}^+ \hat{b}_{\lambda \vec{q}_{\parallel}} + \frac{1}{2}) + \\ &+ \sum_{q_{\perp}, \vec{q}_{\parallel}} \Omega_{L1} (\hat{b}_{q_{\perp} \vec{q}_{\parallel}}^+ \hat{b}_{q_{\perp} \vec{q}_{\parallel}} + \frac{1}{2}) + \\ &+ \sum_{\sigma=S,A} \sum_{p=\pm} \sum_{\vec{q}_{\parallel}} \Omega_{\sigma p}(\vec{q}_{\parallel}) (\hat{b}_{\sigma p \vec{q}_{\parallel}}^+ \hat{b}_{\sigma p \vec{q}_{\parallel}} + \frac{1}{2}). \end{aligned} \quad (17)$$

Here, Ω_{L0} and Ω_{L1} are the energies of longitudinally polarized optical phonons confined “0” and semiconfined in the medium “1”; $\hat{b}_{\lambda \vec{q}_{\parallel}}^+$, $\hat{b}_{\lambda \vec{q}_{\parallel}}$, $\hat{b}_{q_{\perp} \vec{q}_{\parallel}}^+$, and $\hat{b}_{q_{\perp} \vec{q}_{\parallel}}$ are the creation and annihilation operators of the corresponding vibrational states with either discrete ($q_{\lambda} = \lambda\pi/a$; $\lambda = 1, 2, \dots, N$; $N = \text{int}(a/a_0)$; and a_0 being the lattice constant of the medium “0”) or continuous transverse components q_{\perp} of the wave vector $\vec{q} = (\vec{q}_{\parallel}, q_{\perp})$.

The energies $\Omega_{\sigma p}(\vec{q}_{\parallel})$ of interface phonons in high- ($p = +$) and low-energy ($p = -$) states are defined by the dispersion equation

$$\begin{aligned} \Omega_{\sigma \pm}^2(\vec{q}_{\parallel}) &= \frac{1}{2(\varepsilon_{\sigma}^{(0)} + \varepsilon_{\sigma}^{(1)})} \times \\ &\times \left(\left[\varepsilon_{\sigma}^{(0)}(\Omega_{L0}^2 + \Omega_{T1}^2) + \varepsilon_{\sigma}^{(1)}(\Omega_{L1}^2 + \Omega_{T0}^2) \right] \pm \right. \\ &\pm \left. \left(\left[\varepsilon_{\sigma}^{(0)}(\Omega_{L0}^2 - \Omega_{T1}^2) + \varepsilon_{\sigma}^{(1)}(\Omega_{L1}^2 - \Omega_{T0}^2) \right]^2 + \right. \right. \\ &\left. \left. + 4(\Omega_{L1}^2 - \Omega_{L0}^2)(\Omega_{T1}^2 - \Omega_{T0}^2)\varepsilon_{\sigma}^{(0)}\varepsilon_{\sigma}^{(1)} \right)^{1/2} \right), \end{aligned} \quad (18)$$

where $\varepsilon_{\sigma}^{(l)}$ are the \vec{q}_{\parallel} -dependent functions

$$\begin{aligned} \varepsilon_{\sigma}^{(0)} &= \varepsilon_{\infty}^{(0)} [1 \mp \exp(-q_{\parallel} a)], \\ \varepsilon_{\sigma}^{(1)} &= \varepsilon_{\infty}^{(1)} [1 \pm \exp(-q_{\parallel} a)], \quad \sigma = \left\{ \begin{array}{l} S \\ A \end{array} \right\}. \end{aligned} \quad (19)$$

Now, the Hamiltonian of free phonons in our nanosystem is entirely determined.

2.3. Hamiltonian of electron-phonon interaction, with all variables in the occupation-number representation

According to the general theory [16], if the polarization potential of confined phonons is known, the Hamiltonian of interaction between an electron and the quantized phonon field is [5]

$$\hat{H}_{e-LI} = \sum_{q_{\perp}, \vec{q}_{\parallel}} V_{q_{\perp}, \vec{q}_{\parallel}}(z) e^{i\vec{q}_{\parallel} \vec{\rho}} \hat{B}_{q_{\perp}, \vec{q}_{\parallel}}, \quad (20)$$

where

$$\hat{B}_{q_{\perp}, \vec{q}_{\parallel}} = \hat{b}_{q_{\perp}, \vec{q}_{\parallel}} + \hat{b}_{q_{\perp}, -\vec{q}_{\parallel}}^+,$$

$$\begin{aligned} V_{q_{\perp}, \vec{q}_{\parallel}}(z) &= i \sqrt{\frac{4\pi e^2}{\varepsilon_l} \frac{\Omega_{Ll}}{\tilde{S} \tilde{a}_1} \frac{\Omega_{Ll}}{q_{\perp}^2 + q_{\parallel}^2}} \times \\ &\times (1 - \Theta[(-1)^l (|z| - \frac{a}{2})]) \sin[q_{\perp} l (|z| + (-1)^l \frac{a}{2})], \end{aligned} \quad (21)$$

$$\frac{1}{\varepsilon_l} = \frac{1}{\varepsilon_{\infty}^{(l)}} - \frac{1}{\varepsilon_0^{(l)}}, \quad q_{\perp 0} = \frac{\lambda\pi}{a}, \quad q_{\perp 1} = q_{\perp},$$

$$|z|_l = \begin{cases} z, & l = 0; \\ |z|, & l = 1, \end{cases}$$

\tilde{S} is the area of the main region in the XOY plane, $\tilde{a}_0 = a$ is the film thickness, and \tilde{a}_1 is the size of the main region in the half-space $z > a$.

The Hamiltonian of interaction between the electron and the interface phonons looks like

$$\hat{H}_{e-I} = \sum_{\sigma, p, \vec{q}_{\parallel}} V_{\sigma p \vec{q}_{\parallel}}(z) e^{i\vec{q}_{\parallel} \vec{\rho}} \hat{B}_{\sigma p \vec{q}_{\parallel}}, \quad (22)$$

where

$$\hat{B}_{\sigma p \vec{q}_{\parallel}} = \hat{b}_{\sigma p \vec{q}_{\parallel}} + \hat{b}_{\sigma p, -\vec{q}_{\parallel}}^+,$$

$$\begin{aligned} V_{\sigma p \vec{q}_{\parallel}}(z) &= i \sqrt{\frac{\pi e^2 \Omega_{\sigma p}(\vec{q}_{\parallel})}{\varepsilon_{\infty}^{(1)} \tilde{S} q_{\parallel}}} \times \\ &\times \sqrt{\frac{\varepsilon_{\sigma}^{(1)}}{\varepsilon_{\sigma}^{(0)} \zeta_{\sigma p}^{(0)} + \varepsilon_{\sigma}^{(1)} \zeta_{\sigma p}^{(1)}}} I_{\sigma \vec{q}_{\parallel}}(z), \quad \sigma = \left\{ \begin{array}{l} S \\ A \end{array} \right\}, \end{aligned} \quad (23)$$

$$\zeta_{\sigma p}^{(l)} = \frac{\varepsilon_l \Omega_{\sigma p}^2(\vec{q}_{\parallel})}{\varepsilon_0^{(l)} \Omega_{Tl}^2} \left(\frac{\Omega_{Ll}^2 - \Omega_{Tl}^2}{\Omega_{Tl}^2 - \Omega_{\sigma p}^2(\vec{q}_{\parallel})} \right)^2, \quad (24)$$

$$I_{\sigma \vec{q}_{\parallel}}(z) = \begin{cases} \pm e^{q_{\parallel}(z+a/2)}, & z < -\frac{a}{2}; \\ \frac{e^{q_{\parallel}z} \pm e^{-q_{\parallel}z}}{e^{q_{\parallel}a/2} \pm e^{-q_{\parallel}a/2}}, & |z| \leq \frac{a}{2}; \\ e^{-q_{\parallel}(z-a/2)}, & z > \frac{a}{2}, \end{cases} \quad \left(\sigma = \begin{Bmatrix} S \\ A \end{Bmatrix} \right). \quad (25)$$

The changeover to the occupation-number representation in operators (20) and (22) allows the Hamiltonian of electron-phonon interaction to be obtained in the form, where all system variables are expressed in the secondary quantization representation:

$$\begin{aligned} \hat{H}_{e-ph} &= \hat{H}_{e-L0} + \hat{H}_{e-L1} + \hat{H}_{e-I} = \\ &= \sum_{j=d,c} \sum_{n,n',\vec{k}_{\parallel}} \left(\sum_{\lambda,\vec{q}_{\parallel}} F_{nn'}^{\lambda(j)}(\vec{q}_{\parallel}) \hat{a}_{n'\vec{k}_{\parallel}+\vec{q}_{\parallel}}^+ \hat{a}_{n\vec{k}_{\parallel}} \hat{B}_{\lambda\vec{q}_{\parallel}} + \right. \\ &+ \sum_{q_{\perp},\vec{q}_{\parallel}} F_{nn'}^{q_{\perp}(j)}(\vec{q}_{\parallel}) \hat{a}_{n'\vec{k}_{\parallel}+\vec{q}_{\parallel}}^+ \hat{a}_{n\vec{k}_{\parallel}} \hat{B}_{q_{\perp}\vec{q}_{\parallel}} + \\ &\left. + \sum_{\sigma p \vec{q}_{\parallel}} F_{nn'}^{\sigma p(j)}(\vec{q}_{\parallel}) \hat{a}_{n'\vec{k}_{\parallel}+\vec{q}_{\parallel}}^+ \hat{a}_{n\vec{k}_{\parallel}} \hat{B}_{\sigma p \vec{q}_{\parallel}} \right). \quad (26) \end{aligned}$$

Here, the superscript j accepts two values: d corresponds to the discrete and c to the continuous section of the spectrum.

Now, the functions, which describes the coupling between an electron in every state of its discrete spectrum with every branch of the phonon spectrum, are obtained in an explicit analytical form. In particular, for the interaction with confined polarization phonons,

$$\begin{aligned} F_{nn'}^{\lambda(d)}(\vec{q}_{\parallel}) &= i2\lambda \sqrt{\frac{\pi^3 e^2 \Omega_{L0}}{\varepsilon_0 \tilde{S}}} \times \\ &\times \sqrt{\frac{a}{(\lambda\pi)^2 + (aq_{\parallel})^2}} C_n C_{n'} X_{nn'}^{\lambda}, \quad (27) \end{aligned}$$

where

$$X_{nn'}^{\lambda} =$$

$$= \begin{cases} \frac{\cos[(k_{0n} - k_{0n'})a/2]}{(\lambda\pi)^2 - [(k_{0n} - k_{0n'})a]^2} - & (n \cdot n') - \text{even}, \\ -\frac{(-1)^n \cos[(k_{0n} + k_{0n'})a/2]}{(\lambda\pi)^2 - [(k_{0n} + k_{0n'})a]^2} \lambda = 1, 3, \dots; \\ \frac{(-1)^{n-1} \sin[(k_{0n} - k_{0n'})a/2]}{(\lambda\pi)^2 - [(k_{0n} - k_{0n'})a]^2} - & (n \cdot n') - \text{odd}, \\ -\frac{\sin[(k_{0n} + k_{0n'})a/2]}{(\lambda\pi)^2 - [(k_{0n} + k_{0n'})a]^2}, & \lambda = 2, 4, \dots \end{cases} \quad (28)$$

For the interaction with semiconfined polarization phonons,

$$\begin{aligned} F_{nn'}^{q_{\perp}(d)}(\vec{q}_{\parallel}) &= i \frac{4}{a} \sqrt{\frac{\pi e^2 \Omega_{L1} q_{\perp}^2}{\varepsilon_1 \tilde{S} \tilde{a}_1 (q_{\perp}^2 + q_{\parallel}^2)}} \times \\ &\times C_n C_{n'} \frac{\text{cs}(k_{0n}a/2) \text{cs}(k_{0n'}a/2)}{q_{\perp}^2 + (k_{1n} + k_{1n'})^2}, \quad (29) \end{aligned}$$

provided that n and n' are of identical parity. At last, for the interaction with interface phonons,

$$\begin{aligned} F_{nn'}^{\sigma p(d)}(\vec{q}_{\parallel}) &= \frac{i}{a} \sqrt{\frac{\pi e^2 \Omega_{\sigma p}(\vec{q}_{\parallel})}{(\varepsilon_{\sigma}^{(0)} \zeta_{\sigma p}^{(0)} + \varepsilon_{\sigma}^{(1)} \zeta_{\sigma p}^{(1)}) \tilde{S} q_{\parallel}}} \times \\ &\times C_n C_{n'} f_{nn'}^{\sigma p}(\vec{q}_{\parallel}), \quad (30) \end{aligned}$$

where

$$\begin{aligned} f_{nn'}^{\sigma p}(\vec{q}_{\parallel}) &= \sqrt{1 + \exp(-q_{\parallel}a) \delta_{\sigma,S}} \times \\ &\times \left[\text{cs}\left(\frac{k_{0n}a}{2}\right) \text{cs}\left(\frac{k_{0n'}a}{2}\right) \frac{2}{k_{1n} + k_{1n'} + q_{\parallel}} + \right. \\ &+ \sum_{l=0}^1 \frac{(-1)^{(n-1)l}}{(k_{0n} - (-1)^l k_{0n'})^2 + q_{\parallel}^2} \times \\ &\times \left(q_{\parallel} \text{th} \frac{q_{\parallel}a}{2} \cos \frac{(k_{0n} - (-1)^l k_{0n'})a}{2} + \right. \\ &\left. \left. + (k_{0n} - (-1)^l k_{0n'}) \sin \frac{(k_{0n} + (-1)^l k_{0n'})a}{2} \right) \right], \quad (31) \end{aligned}$$

if n and n' are of the same parity, and

$$f_{nn'}^{\sigma p}(\vec{q}_{\parallel}) = \sqrt{1 - \exp(-q_{\parallel}a) \delta_{\sigma,A}} \times$$

$$\begin{aligned}
& \times \left[\text{cs}\left(\frac{k_{0n}a}{2}\right) \text{cs}\left(\frac{k_{0n'}a}{2}\right) \frac{2}{k_{1n} + k_{1n'} + q_{\parallel}} + \right. \\
& + \sum_{l=0}^1 \frac{(-1)^{nl}}{(k_{0n} + (-1)^l k_{0n'})^2 + q_{\parallel}^2} \times \\
& \times \left(q_{\parallel} \text{cth} \frac{q_{\parallel}a}{2} \sin \frac{(k_{0n} + (-1)^l k_{0n'})a}{2} - \right. \\
& \left. \left. - (k_{0n} + (-1)^l k_{0n'}) \cos \frac{(k_{0n} + (-1)^l k_{0n'})a}{2} \right) \right], \quad (32)
\end{aligned}$$

otherwise.

We note that the analytical expressions for the functions of the electron-phonon coupling through states in the continuous range of the electron energy spectrum can be obtained in a similar manner. Since they are cumbersome, they are not displayed here; nevertheless, they will be used while constructing the corresponding mass operator.

Thus, we obtained a Hamiltonian for an electron-phonon system in a flat semiconducting nanofilm located in an external semiconducting medium. It makes it possible to study various theoretical problems concerning the polarization phonon interaction not only with electrons, but with holes and excitons as well.

3. Fourier Transform of the Electron Green's Function and Renormalization of the Main Energy Band by Phonons

To study the renormalization of the main energy band of electrons owing the interaction of the latter with phonons of all types in a nanofilm at $T = 0$ K, we use a Green's function method. According to the general theory of the method [16], the electron Green's function in the energy representation is connected with the total mass operator $M(\vec{k}, E)$ through the Dyson equation

$$G(\vec{k}, E) = [E - E(\vec{k}) - M(\vec{k}, E)]^{-1}. \quad (33)$$

In this work, we confine the consideration to studying the nanosystems with weak electron-phonon coupling. In accordance with the Feynman-Pines technique, it is sufficient to keep only the basic diagram, which corresponds to a one-phonon approximation, in the infinite series of diagrams for the mass operator in order to calculate the renormalization of the main energy band

(without phonon recurrences) [16]. In this case, the mass operator of the system under investigation looks like

$$\begin{aligned}
M(\vec{k}_{\parallel}, E) &= \sum_{\Lambda, \vec{q}_{\parallel}} \frac{|F_{11}^{\Lambda(d)}(\vec{q}_{\parallel})|^2}{E - E_1(\vec{k}_{\parallel} + \vec{q}_{\parallel}) - \Omega_{\Lambda}(\vec{q}_{\parallel})} + \\
&+ \sum_{n \geq 2} \sum_{\Lambda, \vec{q}_{\parallel}} \frac{|F_{1n}^{\Lambda(d)}(\vec{q}_{\parallel})|^2}{E - E_n(\vec{k}_{\parallel} + \vec{q}_{\parallel}) - \Omega_{\Lambda}(\vec{q}_{\parallel})} + \\
&+ \sum_{\Lambda, \vec{q}_{\parallel}} \int_0^{\infty} \frac{|F_{1k_{\perp}}^{\Lambda(c)}(\vec{q}_{\parallel})|^2 d\mathbf{k}_{\perp}}{E - E(k_{\perp}, \vec{k}_{\parallel} + \vec{q}_{\parallel}) - \Omega_{\Lambda}(\vec{q}_{\parallel})}. \quad (34)
\end{aligned}$$

Here, the first summand describes the interaction between the electron and all phonon branches ($\Lambda = \lambda, q_{\perp}, (\sigma, p)$) through the main band states, the second and the third ones through the states of upper bands in the discrete and continuous spectral ranges, respectively. Since the electron-phonon interaction is weak, the mass operator (34) weakly depends on the energy E and the quasimomentum \vec{k} of an electron. Therefore, the shift of the bottom of the main electron band is given by the expression

$$\Delta \equiv M(\vec{k}_{\parallel} = 0, E = E_1) = \Delta_{L0} + \Delta_{L1} + \Delta_I, \quad (35)$$

where Δ_{L0} , Δ_{L1} , and Δ_I are the partial shifts caused by the electron interaction with confined, semiconfined, and interface phonons, respectively. In turn, each of the partial shifts is governed by three mechanisms of interaction between the electrons and phonons: through the states in the main band and in all upper bands in the discrete and continuous sections of the spectrum. Using the corresponding notations $d1$, $d\Sigma$, and c for the contributions made by those mechanisms, we write down

$$\begin{aligned}
\Delta_I &= \Delta_I^{(d1)} + \Delta_I^{(d\Sigma)} + \Delta_I^{(c)}, \\
\Delta_{Ll} &= \Delta_{Ll}^{(d1)} + \Delta_{Ll}^{(d\Sigma)} + \Delta_{Ll}^{(c)}, \quad (l = 0, 1). \quad (36)
\end{aligned}$$

Fulfilling the integration in Eq. (34) over the two-dimensional quasimomentum \vec{q}_{\parallel} and using Eq. (27), we obtain an explicit analytical expression for the shift of the band bottom caused by the interaction between the electron and confined phonons, with engaging all states belonging to the discrete part of the spectrum:

$$\Delta_{L0}^{(d)} = \Delta_{L0}^{(d1)} + \Delta_{L0}^{(d\Sigma)} = \frac{\pi^2 e^2}{a \varepsilon_0} C_1^2 \sum_{n, \lambda} \lambda^2 C_1^2 \Phi_{\lambda}(E_n) |X_{1n}^{\lambda}|^2, \quad (37)$$

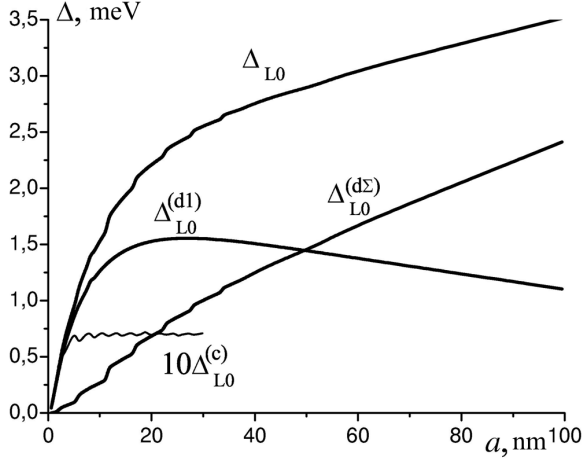


Fig. 2. Dependence of the absolute value of the shift Δ_{L0} of the bottom of the main electron energy band, which occurs owing to the interaction between confined optical polarization phonon and all electron states, on the film thickness a , and the same dependences for the contributions to Δ_{L0} made by the states in the main band ($\Delta_{L0}^{(d1)}$), all other states of the discrete range of the spectrum ($\Delta_{L0}^{(d\Sigma)}$), and the continuous states ($\Delta_{L0}^{(c)}$, thin curve, 10-fold magnification)

where

$$\Phi_\lambda(E) = \ln \frac{\left(\frac{a}{\lambda a_0}\right)^2 + 1}{\left(\frac{a}{a_0}\right)^2 \eta(E) + 1} \left(\lambda^2 \eta(E_1) - \frac{E - E_1}{\Omega_{L0}} - 1 \right)^{-1},$$

$$\eta(E) = \frac{\pi^2 \hbar^2}{2m_0 a^2 (E - E_1 + \Omega_{L0})}. \quad (38)$$

The shifts caused by semiconfined phonons are found analogously:

$$\Delta_{L1}^{(d)} = \Delta_{L1}^{(d1)} + \Delta_{L1}^{(d\Sigma)} = \frac{4e^2}{\pi a^2 \varepsilon_1} C_1^2 \times$$

$$\times \cos^2\left(\frac{k_{01}a}{2}\right) \sum_{n=1,3,\dots} C_n^2 \cos^2\left(\frac{k_{0n}a}{2}\right) \times$$

$$\times \int \frac{\Phi(q_\perp, E_n) q_\perp^2 dq_\perp}{[q_\perp^2 + (k_{1n} + k_{1n'})^2]^2}, \quad (39)$$

where $\Phi(q_\perp, E_n)$ is determined from Eq. (38) with the substitutions $\lambda \rightarrow a q_\perp / \pi$ and $\pi/a \rightarrow q_\perp$.

The partial shift caused by interface phonons is as follows:

$$\Delta_I^{(d)} = \Delta_I^{(d1)} + \Delta_I^{(d\Sigma)} = -\frac{e^2}{2a^2} C_1^2 \times$$

$$\times \sum_n C_n^2 \sum_{\sigma,p} \int dq_\parallel |f_{1n}^{\sigma p}(\vec{q}_\parallel)|^2 \Phi_{\sigma p}(\vec{q}_\parallel) \times$$

$$\times \left[\frac{\hbar^2 q_\parallel^2}{2m_0 \Omega_{\sigma p}(\vec{q}_\parallel)} + \frac{E_n - E_1}{\Omega_{\sigma p}(\vec{q}_\parallel)} + 1 \right]^{-1}, \quad (40)$$

where

$$\Phi_{\sigma p}(\vec{q}_\parallel) = \frac{1}{\Omega_{\sigma p}^2(\vec{q}_\parallel)} \left(\frac{\varepsilon_\sigma^{(0)}(\Omega_{L0}^2 - \Omega_{T0}^2)}{[\Omega_{T0}^2 - \Omega_{\sigma p}^2(\vec{q}_\parallel)]^2} + \right.$$

$$\left. + \frac{\varepsilon_\sigma^{(1)}(\Omega_{L1}^2 - \Omega_{T1}^2)}{[\Omega_{T1}^2 - \Omega_{\sigma p}^2(\vec{q}_\parallel)]^2} \right)^{-1}. \quad (41)$$

The partial shifts caused by the electron-phonon interaction with engaging all continuous states can be determined making use of formulas (37)–(41), where the summation over n is replaced by the integration over the variable k_\perp changing within the interval $(\sqrt{2m_0 V}/\hbar, \infty)$.

4. Analysis of the Results Obtained

The specific calculation for the shift of the bottom of the main band was executed for a β -HgS nanofilm embedded into the β -CdS matrix. For this case, we used the following values taken from work [16] for the physical parameters of the system concerned: $a_0 = 5.851 \text{ \AA}$, $m_0 = 0.036$ and $m_1 = 0.2$ (both in free-electron mass units), $\varepsilon_0^{(0)} = 18.2$, $\varepsilon_\infty^{(0)} = 11.36$, $\varepsilon_0^{(1)} = 9.1$, $\varepsilon_\infty^{(1)} = 5.5$, $V = 1.35 \text{ eV}$, $\Omega_{L0} = 27.8 \text{ meV}$, and $\Omega_{L1} = 57.2 \text{ meV}$.

In Fig. 2, the calculated dependence of the absolute value of the partial shift Δ_{L0} of the bottom of the main electron energy band, induced by the interaction between the electron and confined phonons, on the nanofilm thickness a is depicted, as well as the same dependences for contributions made by the participation of the main band states ($\Delta_{L0}^{(d1)}$) and all other states in the discrete ($\Delta_{L0}^{(d\Sigma)}$) and continuous ($\Delta_{L0}^{(c)}$) spectral ranges in this interaction. One can see that, as far as the film is thin ($a \leq 20 \text{ nm}$), the main contribution to the Δ_{L0} -value is given by the electron-phonon interaction through the main band states, and its magnitude increases with the growth of the film thickness. The total contribution by all upper states in the discrete section of the spectrum is small at small film thicknesses; nevertheless, it also quickly increases as a grows. At $a \approx 25 \text{ nm}$, the values of $\Delta_{L0}^{(d\Sigma)}$ and $\Delta_{L0}^{(d1)}$ become equal.

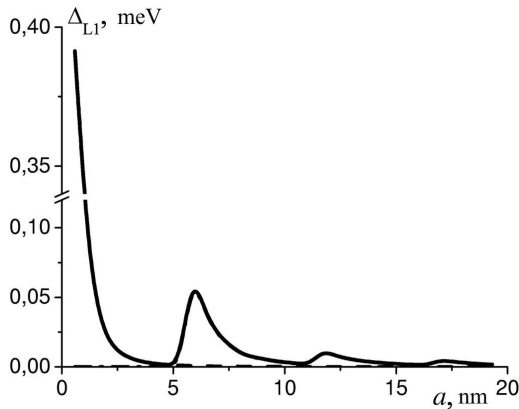


Fig. 3. Dependence of the absolute value of the shift Δ_{L1} of the bottom of the main electron energy band, which occurs owing to the interaction between semiconfined optical polarization phonons and all electron states, on the film thickness a , and the same dependences for the contributions to Δ_{L1} made by the states in the main band ($\Delta_{L1}^{(d1)}$, dashed curve) and all other states of the discrete range of the spectrum ($\Delta_{L1}^{(d\Sigma)}$, dotted curve)

A further growth of the film thickness leads to a smooth reduction of the shift caused by the interaction with the main band states, while the total contribution of the upper states increases at that.

The contribution by continuous states first drastically increases when a grows up to 5 nm; then it reaches, by weakly oscillating, a saturation level, the value of which does not exceed 4–5% of $\Delta_{L0}^{(d1)}$. The total partial shift Δ_{L0} occurring owing to the interaction with confined phonons monotonously increases with the growth of the film thickness and saturates at 3.4 meV for $a \geq 100$ nm.

In Fig. 3, the dependences of the absolute value of the partial bottom shift Δ_{L1} and its components on the film thickness a are exhibited. The figure demonstrates that the intraband interaction ($\Delta_{L1}^{(d1)}$) makes a dominant contribution to the formation of the Δ_{L0} -value. The total contribution of the interband interaction through states of the discrete spectral range ($\Delta_{L1}^{(d\Sigma)}$) is small, and that through continuous states ($\Delta_{L1}^{(c)}$) does not exceed one percent of $\Delta_{L1}^{(d1)}$ and, therefore, is not shown in the figure.

A fast reduction of the Δ_{L1} -magnitude, which accompanies the growth of the film thickness a , is connected with the fact that, in this case, the bottom of the electron energy band goes down in the quantum well proportionally to a^{-2} , which is equivalent to a drastic increase of the effective power of the potential barrier.

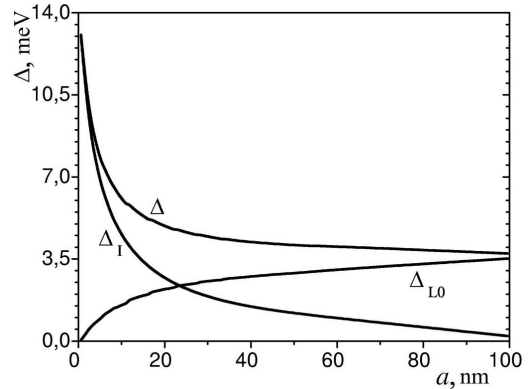


Fig. 4. Dependences of the absolute values of the shifts of the bottom of the main electron energy band, which occur owing to the interaction with interface (Δ_I) and confined (Δ_{L0}) phonons, and of the total shift $\Delta = \Delta_{L0} + \Delta_I$ on the film thickness a

This circumstance gives rise to a decrease of the probability for an electron to penetrate into the environment and, hence, reduces the magnitude of the corresponding electron-phonon interaction.

The peaks observed in the plot of the dependence of $\Delta_{L1}^{(d\Sigma)}$ on a are caused by the contributions made by the symmetric-state bands in the discrete part of the electron spectrum (with odd n numbers) as they emerge in turn in the quantum well as the width of the latter grows.

The calculation of the partial shift Δ_I resulted from the interaction with interface phonons showed that an electron from the main band does not interact with the antisymmetric branch of interface phonons, because the wave function of the former is symmetric, so that the interaction through states in the upper bands of the discrete section of the spectrum makes a contribution that does not exceed 0.4% of the $\Delta_I^{(d1)}$ -magnitude. The contribution of states from the continuous part of the spectrum is negligibly small. Therefore, the dominant contribution to the shift of the main band bottom Δ_I is made by the intraband interaction with the symmetric branch of interface phonons.

In Fig. 4, the dependences of the absolute values of the partial, Δ_{L0} and Δ_I , and total, $\Delta = \Delta_{L0} + \Delta_I$, shifts on the nanofilm thickness a are depicted. It is evident that the shift of the bottom of the main band in thin films ($a < 25$ nm) is mainly governed by the interaction with interface phonons, and – as the film thickness increases – with confined ones. If the film thickness increases substantially, the influence of interface phonons vanishes, and the magnitude of Δ_{L0} approaches the value $\Delta^{3D} = 3.9$ meV characteristic of a

massive β -HgS crystal. Such a behavior can be entirely understood, because, as the film thickness increases, the probability to find an electron at the heterojunction interfaces decreases, while the probability to find it in the quantum well region increases.

The general conclusions of the work are as follows. An explicit analytical expression for the Hamiltonian, which describes the electron-phonon system of a nanofilm surrounded by a semiconducting medium and all the variables of which are given in the occupation-number representation, has been obtained for the first time. This made it possible to apply the Green's function method to calculate the position of the bottom of the main electron band renormalized by the electron-phonon interaction. The contributions of all mechanisms of the electron-phonon interaction have been analyzed in detail. The mechanism of the intraband interaction with the symmetric branch of interface phonons has been demonstrated to be dominating in thin films, while – in the thick-film case – it is the interaction of all states of the discrete part of the electron energy spectrum with confined phonons that prevails; this conclusion completely correlates with similar conclusions drawn for other methods and other systems [4,5]. An advantage of the Green's function method applied here consists in that it allows one, in contrast to other theoretical methods, to study the renormalization of an arbitrary electron energy band, for an arbitrary magnitude of electron-phonon coupling, at $T \neq 0$ K, and in a wide energy range which includes electron-phonon recurrences. This task will be dealt with in the following works.

1. Zh.I. Alferov, *Fiz. Tekh. Poluprovodn.* **32**, 3 (1998).
2. K. Huang and B.F. Zhu, *Phys. Rev. B* **38**, 13377 (1988).
3. N. Mori and T. Ando, *Phys. Rev. B* **40**, 6175 (1989).
4. R. Zheng and M. Matsuura, *Phys. Rev. B* **57**, 1749 (1998).
5. G.Q. Hai, F.M. Peeters, and J.T. Devreese, *Phys. Rev. B* **48**, 4666 (1993).
6. B. Zhu, *Phys. Rev. B* **44**, 1926 (1991).
7. W.S. Li and C.Y. Chen, *Physica B* **229**, 375 (1997).

8. N.V. Tkach and V.P. Zharkoi, *Fiz. Tekh. Poluprovodn.* **33**, 598 (1999).
9. N.V. Tkach, *Fiz. Tverd. Tela* **39**, 1109 (1997).
10. M. Tkach, V. Holovatsky, O. Voitsekhivska *et al.*, *Phys. Status Solidi B* **203**, 373 (1997).
11. B. El Amrani, M. Fliyou, M. Barnoussi *et al.*, *Phys. Status Solidi B* **219**, 39 (2000).
12. V.I. Boichuk and V.A. Borusevych, *Ukr. J. Phys.* **51**, 169 (2006).
13. A.V. Novikov, A.B. Andreev, N. Vostokov *et al.*, *Mater. Sci. Eng. B* **89**, 62 (2002).
14. D. Schoos, A. Mews, A. Eychmuller *et al.*, *Phys. Rev. B* **49**, 17072 (1994).
15. V.I. Boichuk and D.J. Kubai, *Fiz. Tverd. Tela* **43**, 226 (2001).
16. M.V. Tkach, *Quasiparticles in Nanoheterosystems. Quantum Dots and Wires* (Chernivtsi Nat. Univ. Publ. House, Chernivtsi, 2003) (in Ukrainian).

Received 26.12.07.

Translated from Ukrainian by O.I. Voitenko

ЕЛЕКТРОН-ФОНОННА ВЗАЄМОДІЯ І МЕХАНІЗМИ ПЕРЕНОРМУВАННЯ ЕЛЕКТРОННОГО ЕНЕРГЕТИЧНОГО СПЕКТРА ПЛОСКОЇ НАНОПЛІВКИ

М.В. Ткач, В.М. Крамар

Р е з ю м е

У моделі діелектричного континууму для фононів та прямокутних потенціалів і ефективних мас – для електронів, отримано гамільтоніан електрон-фононної взаємодії у зображенні чисел заповнення за всіма змінними системи для плоскої напівпровідникової плівки (потенціальної ями), розташованої у напівпровідниковому середовищі. Методом функцій Гріна виконано аналітичний розрахунок перенормованого фононами положення дна основної електронної зони. На прикладі плоскої наногетеросистеми β -HgS/ β -CdS виконано числовий розрахунок зміщення дна зони при $T = 0$ К. Проаналізовано внески у величину зміщення всіх можливих механізмів електрон-фононної взаємодії. Показано, що у випадку тонких наноплівок зміщення формується внутрішньозонною взаємодією електрона з симетричною модою інтерфейсних фононів. У випадку товстих наноплівок домінуючою стає взаємодія електрона з просторово обмеженими фононами за участі всіх зон дискретної частини енергетичного спектра.