

THERMAL GENESIS OF THE BOTTOM OF MAIN ELECTRON'S ENERGY BAND IN A FLAT NANOFILM

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In the approximation of a dielectric continuum for phonons and in the approximation of rectangular potentials and effective masses for electrons, the analytic calculation of a position of the bottom of the main electron's energy band renormed by phonons in a plane quantum well (a semiconductor film) placed in the external semiconductor medium is carried out by the Green's function method. By the example of a plane nanoheterosystem β -HgS/ β -CdS, the shift of the electron's band bottom as a function of both the film thickness and the temperature is numerically calculated. It is shown that, as the temperature grows, the electron-phonon interaction in the processes of absorption and emission leads to a shift of the band bottom to the region of lower energies. The mechanisms of the increase in the shift with the temperature in films with various thicknesses, as well as the reasons for different shift rates of the electron's band bottom with increase in the temperature, are established.

points [9–11] created on the basis of heterojunctions in semiconductor media was theoretically studied mainly in the approximation of dielectric continuum for the phonon subsystem and in the model of rectangular potentials and effective masses for an electron, hole, or exciton.

In particular, the problem concerning the study of structural changes of the electron spectrum due to the interaction with phonons in planar semiconductor nanofilms was solved by the method of perturbation theory [3, 5] or within the Lee–Low–Pines variation method [12]. The above-mentioned and similar works have mainly considered the nanosystems with weak electron-phonon coupling at $T = 0$ K, and the Hamiltonian of the system was written in the representation of occupation numbers in phonon variables and in the coordinate representation in electron variables. The applied methods allowed one to study the role of the electron-phonon interaction in changes of the ground-state energy and the effective masses of free carriers due to a variation in the nanofilm thickness.

The mentioned approaches do not allow one to investigate the systems with intermediate and strong electron-phonon couplings. They cannot be applied also to the study of processes at $T > 0$ K, which is of importance, for example, for the account of electron- and exciton-phonon recurrences in nanosystems, whereas the phenomenon of Raman scattering in these systems has been experimentally already studied [13]. Hence, one needs to construct a sequential theory of electron- and exciton-phonon interactions which would explain various phenomena in low-dimension nanostructures with arbitrary coupling strength, in a wide interval of energies, and at arbitrary temperatures of the

1. Introduction

In the last decades, the studies in the field of solid state physics are mainly directed to the clarification of properties of quantum-sized nanosystems. The energy spectra of electrons, holes, and excitons, and phonons in semiconductor nanosystems are studied, because they allow one to establish the regularities of a course of various phenomena which are promising, in particular, from the viewpoint of their practical applications [1]. The interaction between quasiparticles causes a change in spectra, which is directly manifested in a change in physical parameters of quantum-sized systems and devices fabricated on their basis. Therefore, the development of the theory of the interaction of quasiparticles between one another and with external fields remains a topical task.

The interaction of phonons with free carriers and excitons in quantum wells [2–5], wires [6–8], and

system. The first attempt in this direction [14] was completed by the construction of the Hamiltonian of the electron-phonon system in a semiconductor nanofilm in the representation of occupation numbers in all variables of the system, which allowed one to study the interaction of various phonon states with free carriers and excitons on the basis of the universal method of Green's functions at $T = 0$ K.

The main purpose of the present work is the expansion of studies of the electron-phonon interaction in plane quantum wells (nanofilms) onto real systems at arbitrary temperatures ($T \neq 0$ K). In particular, we will obtain the analytic formula for a shift of the bottom of the main electron's energy band as a function of the temperature and film thickness. The specific calculations were carried out by the example of a planar nanofilm β -HgS in the β -CdS medium which can be obtained experimentally [15].

It is shown that the account of the electron-phonon interaction accompanied both by absorption and with emission of phonons at $T > 0$ K leads to a complicated temperature dependence of the shift of the band bottom at various film thicknesses. We will also determine the contributions of various mechanisms of the formation of a temperature shift of the band bottom in films with various thicknesses.

2. Hamiltonian of the Electron-Phonon System in a Planar Nanofilm. The Representation of Secondary Quantization

Let us consider an electron in a planar semiconductor nanofilm (quantum well) positioned in a massive semiconductor medium. We choose the Cartesian coordinate system so that its origin was located at the middle of the film with thickness a and take the XOY plane to be parallel to its surface. Since we study the nanoheterosystem with small differences of the lattice constants ($a_0 = 5.851$ Å, and $a_1 = 5.818$ Å) and dielectric permittivities ($\varepsilon_0^{(0)} = 18.2$; $\varepsilon_\infty^{(0)} = 11.36$; $\varepsilon_0^{(1)} = 9.1$; $\varepsilon_\infty^{(1)} = 5.5$) of its components (here and below, the characteristics of a film material and the barrier medium are denoted, respectively, by indices 0 and 1), we neglect the forces of interaction of an electron with electrostatic images [16] and use the approximations of effective mass and rectangular potential barriers with finite heights.

Thus, we assume that the effective mass $m(z)$ and the potential energy of an electron $V(z)$ are known:

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

Using the solutions of the stationary Schrödinger equation given in [5, 6] for the system of free electrons in a nanofilm, we can give the Hamiltonian for a free electron in the representation of secondary quantization as

$$\hat{H}_e = \sum_{\mathbf{k}_\parallel} \left[\sum_n E_n(\mathbf{k}_\parallel) \hat{a}_{n\mathbf{k}_\parallel}^+ \hat{a}_{n\mathbf{k}_\parallel} + \sum_{k_\perp} E(\mathbf{k}_\parallel, k_\perp) \hat{a}_{k_\perp\mathbf{k}_\parallel}^+ \hat{a}_{n\mathbf{k}_\parallel} \right], \quad (2)$$

where $\hat{a}_{n\mathbf{k}_\parallel}^+$ ($\hat{a}_{n\mathbf{k}_\parallel}$) and $\hat{a}_{k_\perp\mathbf{k}_\parallel}^+$ ($\hat{a}_{k_\perp\mathbf{k}_\parallel}$) are the operators of creation (annihilation) of electronic states from the discrete and continual regions of the energy spectrum, respectively.

The energies of electron states in a quantum well

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

are determined by the corresponding quantum number n and the longitudinal component of the wave vector in the quantum well $\mathbf{k}_\parallel = k_x \mathbf{n}_x + k_y \mathbf{n}_y$. The energy $E_n < V$ and is a solution of the dispersion equation

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

((+) at odd and (−) at even values of n).

The wave functions of the symmetric (odd n) and antisymmetric (even n) electron states contain the normalizing factors

$$C_n = \sqrt{2} \left[1 + (-1)^{n-1} \frac{\sin(k_{0n}a)}{k_{0n}a} + 2 \frac{\cos^2(k_{0n}/2)}{k_{1n}a} \right]^{-1/2} \quad (5)$$

and the transverse components of the quasimomenta

$$k_{0n} = \frac{\sqrt{2m_0 E_n}}{\hbar}, \quad k_{1n} = \frac{\sqrt{2m_1(V - E_n)}}{\hbar}. \quad (6)$$

Here and below, we use the functions

$$\begin{aligned} \operatorname{cs}(x_n) &= \begin{cases} \cos x_n, \\ \sin x_n, \end{cases} \\ \operatorname{sc}(x_n) &= \begin{cases} \sin x_n, & n = 1, 3, \dots; \\ \cos x_n, & n = 2, 4, \dots, \end{cases} \end{aligned}$$

which compactify awkward mathematical formulas.

The energies

$$E(\mathbf{k}_{\parallel}, k_{\perp}) = V + \frac{\hbar^2}{2m_0}(k_{\parallel}^2 + k_{\perp}^2) \quad (7)$$

and wave functions of states of the continual region of the electronic spectrum ($E > V$) are also defined by the longitudinal $\mathbf{k}_{0\parallel}$ and transverse ($k_{0\perp} = \sqrt{2m_0E}/\hbar$ in a quantum well and $k_{1\perp} = \sqrt{2m_1(E-V)}/\hbar$ in the barrier medium) components of the wave vector of an electron. States in this part of the spectrum possess also different symmetries [5, 6] and therefore differ from one another by normalizing factors

$$C^{\pm} = \sqrt{2} \left[\text{cs}^2 \left(\frac{k_{0\perp}a}{2} \right) + \frac{m_1E}{m_0(E-V)} \text{sc}^2 \left(\frac{k_{0\perp}a}{2} \right) \right]^{-1/2}, \quad (8)$$

where (+) and (−) are the indices of the symmetric and antisymmetric states, respectively.

In the model of dielectric continuum [5], the Hamiltonian of free phonons in a nanosystem can be represented in the form

$$\begin{aligned} \hat{H}_{\text{ph}} = & \hat{H}_{L0} + \hat{H}_{L1} + \hat{H}_I = \sum_{\lambda, \mathbf{q}_{\parallel}} \Omega_{L0} (\hat{b}_{\lambda \mathbf{q}_{\parallel}}^+ \hat{b}_{\lambda \mathbf{q}_{\parallel}} + \frac{1}{2}) + \\ & + \sum_{q_{\perp}, \mathbf{q}_{\parallel}} \Omega_{L1} (\hat{b}_{q_{\perp} \mathbf{q}_{\parallel}}^+ \hat{b}_{q_{\perp} \mathbf{q}_{\parallel}} + \frac{1}{2}) + \\ & + \sum_{\sigma=S, A} \sum_{p=\pm} \sum_{\mathbf{q}_{\parallel}} \Omega_{\sigma p} (\mathbf{q}_{\parallel}) (\hat{b}_{\sigma p \mathbf{q}_{\parallel}}^+ \hat{b}_{\sigma p \mathbf{q}_{\parallel}} + \frac{1}{2}), \end{aligned} \quad (9)$$

where Ω_{L0} (Ω_{L1}) are the energies of longitudinal optical polarization phonons bounded in medium “0” (semibounded in medium “1”), and $\hat{b}_{\lambda \mathbf{q}_{\parallel}}^+$, $\hat{b}_{q_{\perp} \mathbf{q}_{\parallel}}^+$ ($\hat{b}_{\lambda \mathbf{q}_{\parallel}}$, $\hat{b}_{q_{\perp} \mathbf{q}_{\parallel}}$) are the operators of creation (annihilation) of the corresponding oscillatory states with discrete ($q_{\parallel} = \lambda\pi/a$; $\lambda = 1, 2, \dots, N$; $N = f(a/a_0)$, where a_0 is the lattice constant of medium “0”) or continuous ($q_{\perp}$) transverse components of the wave vector $\mathbf{q} = (\mathbf{q}_{\parallel}, q_{\perp})$.

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

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

$$\begin{aligned} & \left. \pm ([\varepsilon_{\sigma}^{(0)}(\Omega_{L0}^2 - \Omega_{T1}^2) + \varepsilon_{\sigma}^{(1)}(\Omega_{L1}^2 - \Omega_{T0}^2)]^2 + \right. \\ & \left. + 4(\Omega_{L1}^2 - \Omega_{L0}^2)(\Omega_{T1}^2 - \Omega_{T0}^2)\varepsilon_{\sigma}^{(0)}\varepsilon_{\sigma}^{(1)})^{1/2} \right), \end{aligned} \quad (10)$$

where $\varepsilon_{\sigma}^{(l)}$ ($l = 0, 1$) are the functions

$$\varepsilon_{\sigma}^{(l)} = \varepsilon_{\infty}^{(l)} [1 \mp (-1)^l \exp(-q_{\parallel}a)], \quad \sigma = \begin{Bmatrix} S \\ A \end{Bmatrix}, \quad (11)$$

dependent on $\mathbf{q}_{\parallel}$. After the passage to the representation of occupation numbers for all variables, the Hamiltonian of the electron-phonon interaction for a plane quantum well obtained in [5, 6] takes the form

$$\begin{aligned} \hat{H}_{e-\text{ph}} = & \hat{H}_{e-L0} + \hat{H}_{e-L1} + \hat{H}_{e-I} = \\ = & \sum_{j=d, c} \sum_{n, n', \mathbf{k}_{\parallel}} \left(\sum_{\lambda, \mathbf{q}_{\parallel}} F_{nn'}^{\lambda(j)}(\mathbf{q}_{\parallel}) \hat{a}_{n' \mathbf{k}_{\parallel} + \mathbf{q}_{\parallel}}^+ \hat{a}_{n \mathbf{k}_{\parallel}} \hat{B}_{\lambda \mathbf{q}_{\parallel}} + \right. \\ & + \sum_{q_{\perp}, \mathbf{q}_{\parallel}} F_{nn'}^{q_{\perp}(j)}(\mathbf{q}_{\parallel}) \hat{a}_{n' \mathbf{k}_{\parallel} + \mathbf{q}_{\parallel}}^+ \hat{a}_{n \mathbf{k}_{\parallel}} \hat{B}_{q_{\perp} \mathbf{q}_{\parallel}} + \\ & \left. + \sum_{\sigma p \mathbf{q}_{\parallel}} F_{nn'}^{\sigma p(j)}(\mathbf{q}_{\parallel}) \hat{a}_{n' \mathbf{k}_{\parallel} + \mathbf{q}_{\parallel}}^+ \hat{a}_{n \mathbf{k}_{\parallel}} \hat{B}_{\sigma p, \mathbf{q}_{\parallel}} \right), \end{aligned} \quad (12)$$

where the index j distinguishes discrete ($j = d$) and continual ($j = c$) states, $\hat{B}_{\Lambda, \mathbf{q}_{\parallel}} = \hat{b}_{\Lambda, \mathbf{q}_{\parallel}} + \hat{b}_{\Lambda, -\mathbf{q}_{\parallel}}^+$, and $F_{nn'}^{\Lambda(j)}$ are the functions of the coupling of an electron in the n -th band with a phonon of the corresponding branch of oscillations ($\Lambda = \lambda, q_{\perp}, (\sigma, p)$) through states of the n' -th band; their analytic expressions were obtained in [14]. They look as follows:

– the functions of the coupling of an electron with polarization oscillations of atoms of semibounded medium “1” are

$$\begin{aligned} F_{nn'}^{q_{\perp}(d)}(\mathbf{q}_{\parallel}) = & i \frac{4}{a} \sqrt{\frac{\pi e^2 \Omega_{L1} q_{\perp}^2}{\varepsilon_1 \tilde{S} \tilde{a}_1 (q_{\perp}^2 + q_{\parallel}^2)}} \times \\ & \times C_n C_{n'} \frac{\text{cs}(k_{0n}a/2) \text{cs}(k_{0n'}a/2)}{q_{\perp}^2 + (k_{1n} + k_{1n'})^2}, \end{aligned} \quad (13)$$

if n and n' have the same parity;

– the functions of the coupling of an electron with polarization oscillations of atoms of bounded medium "0" are

$$F_{nn'}^{\lambda(d)}(\mathbf{q}_{\parallel}) = i2\lambda \sqrt{\frac{\pi^3 e^2 \Omega_{L0}}{\varepsilon_0 \tilde{S}}} \times \sqrt{\frac{a}{(\lambda\pi)^2 + (aq_{\parallel})^2}} C_n C_{n'} X_{nn'}^{\lambda}, \quad (14)$$

where

$$X_{nn'}^{\lambda} = \begin{cases} \frac{\cos[(k_{0n} - k_{0n'})a/2]}{(\lambda\pi)^2 - [(k_{0n} - k_{0n'})a]^2} - \frac{(-1)^n \cos[(k_{0n} + k_{0n'})a/2]}{(\lambda\pi)^2 - [(k_{0n} + k_{0n'})a]^2}, & (n \cdot n')\text{--even}, \\ \frac{(-1)^{n-1} \sin[(k_{0n} - k_{0n'})a/2]}{(\lambda\pi)^2 - [(k_{0n} - k_{0n'})a]^2} - \frac{\sin[(k_{0n} + k_{0n'})a/2]}{(\lambda\pi)^2 - [(k_{0n} + k_{0n'})a]^2}, & (n \cdot n')\text{--odd}, \\ \frac{\sin[(k_{0n} + k_{0n'})a/2]}{(\lambda\pi)^2 - [(k_{0n} + k_{0n'})a]^2}, & \lambda = 2, 4, \dots; \end{cases} \quad (15)$$

$1/\varepsilon_l = 1/\varepsilon_{\infty} - 1/\varepsilon_0^{(l)}$ ($l = 0, 1$), $\tilde{a}_1$ is the size of the basic domain of medium "1" in the direction of the OZ -axis; $\tilde{S}$ is the area of the basic domain of a crystal in the XOY plane;

– the functions of the coupling of an electron with interface phonons

$$F_{nn'}^{\sigma p(d)}(\mathbf{q}_{\parallel}) = \frac{i}{a} \sqrt{\frac{\pi e^2 \Omega_{\sigma p}(\mathbf{q}_{\parallel})}{(\varepsilon_{\sigma}^{(0)} \zeta_{\sigma p}^{(0)} + \varepsilon_{\sigma}^{(1)} \zeta_{\sigma p}^{(1)}) \tilde{S} q_{\parallel}}} C_n C_{n'} f_{nn'}^{\sigma p}(\mathbf{q}_{\parallel}), \quad (16)$$

where

$$f_{nn'}^{\sigma p}(\mathbf{q}_{\parallel}) = \sqrt{1 + \exp(-q_{\parallel} a)} \delta_{\sigma, S} \times \left[\text{cs}\left(\frac{k_{0n} a}{2}\right) \text{cs}\left(\frac{k_{0n'} a}{2}\right) \frac{2}{k_{1n} + k_{1n'} + q_{\parallel}} + \sum_{m=0}^1 \frac{(-1)^{(n-1)m}}{(k_{0n} - (-1)^m k_{0n'})^2 + q_{\parallel}^2} \times \left(q_{\parallel} \text{th} \frac{q_{\parallel} a}{2} \cos \frac{(k_{0n} - (-1)^m k_{0n'}) a}{2} + \right. \right.$$

$$\left. + (k_{0n} - (-1)^m k_{0n'}) \sin \frac{(k_{0n} + (-1)^m k_{0n'}) a}{2} \right), \quad (17)$$

if n and n' have the same parity, and

$$f_{nn'}^{\sigma p}(\mathbf{q}_{\parallel}) = \sqrt{1 - \exp(-q_{\parallel} a)} \delta_{\sigma, A} \times \left[\text{cs}\left(\frac{k_{0n} a}{2}\right) \text{cs}\left(\frac{k_{0n'} a}{2}\right) \frac{2}{k_{1n} + k_{1n'} + q_{\parallel}} + \sum_{m=0}^1 \frac{(-1)^{nm}}{(k_{0n} + (-1)^m k_{0n'})^2 + q_{\parallel}^2} \times \left(q_{\parallel} \text{cth} \frac{q_{\parallel} a}{2} \sin \frac{(k_{0n} + (-1)^m k_{0n'}) a}{2} - \right. \right. \\ \left. \left. - (k_{0n} + (-1)^m k_{0n'}) \cos \frac{(k_{0n} + (-1)^m k_{0n'}) a}{2} \right) \right], \quad (18)$$

if n and n' have different parities.

Knowing the Hamiltonian of the electron-phonon system for a plane semiconductor nanofilm positioned in the external semiconductor medium, we can study various problems of the theory of the interaction of electrons with polarization phonons. In this work, we present the results of calculations and analysis of the dependence of a position of the main electron's energy band bottom on the temperature and geometric parameters of the CdS/HgS/CdS nanosystem.

3. Renormalization of a Position of the Main Electron's Energy Band Bottom by Phonons at $T \neq 0$ K

We will study the renormalization of the main electron's energy band due to its interaction with phonons in a nanofilm on variations of the temperature by using the method of Green's functions. According to the general theory [17], the Green's function of an electron in the energy representation $G(\mathbf{k}, E)$ is related to the full mass operator $M(\mathbf{k}, E)$ via the Dyson equation

$$G(\mathbf{k}, E) = [E - E(\mathbf{k}) - M(\mathbf{k}, E)]^{-1}. \quad (19)$$

By restricting ourselves to the study of nanosystems with weak electron-phonon coupling at $T \neq 0$ K, we use the one-phonon approximation [17] for the mass operator

$$M(\mathbf{k}_{\parallel}, E, T) = \sum_{\Lambda, \mathbf{q}_{\parallel}} \left(\sum_n |F_{1n}^{\Lambda(d)}(\mathbf{q}_{\parallel})|^2 \times \right.$$

$$\begin{aligned}
& \times \left[\frac{1 + \nu_\Lambda(\mathbf{q}_\parallel, T)}{E - E_n(\mathbf{k}_\parallel - \mathbf{q}_\parallel) - \Omega_\Lambda(\mathbf{q}_\parallel)} + \right. \\
& \left. + \frac{\nu_\Lambda(\mathbf{q}_\parallel, T)}{E - E_n(\mathbf{k}_\parallel + \mathbf{q}_\parallel) + \Omega_\Lambda(\mathbf{q}_\parallel)} \right] + \int_0^{\pi/a} dk_\perp |F_{1k_\perp}^{\Lambda(c)}(\mathbf{q}_\parallel)|^2 \times \\
& \times \left[\frac{1 + \nu_\Lambda(\mathbf{q}_\parallel, T)}{E - E(k_\perp, \mathbf{k}_\parallel - \mathbf{q}_\parallel) - \Omega_\Lambda(\mathbf{q}_\parallel)} + \right. \\
& \left. + \frac{\nu_\Lambda(\mathbf{q}_\parallel, T)}{E - E(k_\perp, \mathbf{k}_\parallel + \mathbf{q}_\parallel) + \Omega_\Lambda(\mathbf{q}_\parallel)} \right], \quad (20)
\end{aligned}$$

where $\nu_\Lambda(\mathbf{q}_\parallel, T) = [\exp(\Omega_\Lambda(\mathbf{q}_\parallel)/k_B T) - 1]^{-1}$ are the mean values of the occupation numbers of the relevant phonon states at the temperature T .

For the systems with weak electron-phonon interaction, the mass operator (20) weakly depends on the energy E and the quasimomentum $\mathbf{k}$ of an electron. Therefore, the shifts of the main electron's energy band bottom can be presented in the form of a function of the temperature T and the nanofilm thickness a as

$$\begin{aligned}
\Delta(a, T) & \equiv M(\mathbf{k}_\parallel = 0, E = E_1, T) = \\
& = \Delta_{L0}(a, T) + \Delta_{L1}(a, T) + \Delta_I(a, T), \quad (21)
\end{aligned}$$

where $\Delta_\Lambda(a, T)$ are the partial shifts caused by the interaction with bounded ($\Lambda = L0$), semibounded ($\Lambda = L1$), and interface ($\Lambda = I$) phonons, respectively. Each of the partial shifts $\Delta_\Lambda(a, T)$, is formed in turn, by three mechanisms of the interaction of an electron with phonons: a) through states of the main ($d1$) band itself, b) through states of all higher bands of the discrete ($d\Sigma$) and c) continual (c) parts of the spectrum:

$$\begin{aligned}
\Delta_\Lambda(a, T) & = \Delta_\Lambda^{(d1)}(a, T) + \Delta_\Lambda^{(d\Sigma)}(a, T) + \\
& + \Delta_\Lambda^{(c)}(a, T) = \Delta_\Lambda^{(d)}(a, T) + \Delta_\Lambda^{(c)}(a, T).
\end{aligned}$$

The shifts $\Delta_{L0}^{(d)}(a, T)$ of the main band bottom caused by the interaction of an electron with bounded $L0$ -phonons with participation of all states of the discrete part of the spectrum can be presented in the form

$$\Delta_{L0}^{(d)}(a, T) = -\frac{\pi^2 e^2}{\varepsilon_0 a} C_1^2 \sum_n C_n^2 \sum_{\lambda=1}^N \lambda^2 \times$$

$$\times |X_{1n}^\lambda|^2 ([1 + \nu_\Lambda(T)] \Phi_{\lambda n}^{(+)} + \nu_\Lambda(T) \Phi_{\lambda n}^{(-)}), \quad (22)$$

where

$$\Phi_{\lambda n}^{(\pm)} = \frac{\ln \frac{\eta + \xi_n \pm 1}{|1 \pm \xi_n|[(N/\lambda)^2 + 1]}}{(\lambda/N)^2 \eta - \xi_n \mp 1}, \quad (23)$$

$$\eta(E) = \frac{\pi^2 \hbar^2}{2m_0 a_0^2 \Omega_{L0}}, \quad \xi_n = \frac{E_n - E_1}{\Omega_{L0}}. \quad (24)$$

Analogously, we determined the shift caused by the interaction of an electron with interface phonons as

$$\begin{aligned}
\Delta_I^{(d)}(a, T) & = -\frac{e^2 C_1^2}{2a^2} \sum_n C_n^2 \times \\
& \times \sum_{\sigma, p=\pm} \left(\int_0^{\pi/a_0} [1 + \nu_{\sigma p}(\mathbf{q}_\parallel, T)] \times \right. \\
& \times \frac{|f_{1n}^{\sigma p}(\mathbf{q}_\parallel)|^2 \Phi_{\sigma p}(\mathbf{q}_\parallel) d\mathbf{q}_\parallel}{\tilde{\eta}_{\sigma p}(\mathbf{q}_\parallel) + \tilde{\xi}_{n\sigma p}(\mathbf{q}_\parallel) + 1} + \\
& \left. + \int_0^{\pi/a_0} \frac{\nu_{\sigma p}(\mathbf{q}_\parallel, T) |f_{1n}^{\sigma p}(\mathbf{q}_\parallel)|^2 \Phi_{\sigma p}(\mathbf{q}_\parallel) d\mathbf{q}_\parallel}{\tilde{\eta}_{\sigma p}(\mathbf{q}_\parallel) + \tilde{\xi}_{n\sigma p}(\mathbf{q}_\parallel) - 1} \right), \quad (25)
\end{aligned}$$

where

$$\begin{aligned}
\Phi_{\sigma p}(\mathbf{q}_\parallel) & = \frac{1}{\Omega_{\sigma p}^2(\mathbf{q}_\parallel)} \left[\frac{\varepsilon_\sigma^{(0)}(\Omega_{L0}^2 - \Omega_{T0}^2)}{[\Omega_{T0}^2 - \Omega_{\sigma p}^2(\mathbf{q}_\parallel)]^2} + \right. \\
& \left. + \frac{\varepsilon_\sigma^{(1)}(\Omega_{L1}^2 - \Omega_{T1}^2)}{[\Omega_{T1}^2 - \Omega_{\sigma p}^2(\mathbf{q}_\parallel)]^2} \right]^{-1}, \quad (26)
\end{aligned}$$

$$\tilde{\eta}_{\sigma p}(\mathbf{q}_\parallel) = \frac{\hbar^2 q_\parallel^2}{2m_0 \Omega_{\sigma p}(\mathbf{q}_\parallel)}, \quad \tilde{\xi}_{n\sigma p} = \frac{E_n - E_1}{\Omega_{\sigma p}(\mathbf{q}_\parallel)}. \quad (27)$$

We give no explicit analytic formulas for the partial shifts $\Delta_{L1}^{(j)}(a, T)$ ($j = d, c$) caused by the interaction of an electron with semibounded phonons, as well as with $L0$ - and I -phonons through states of the continual part of the spectrum, because the corresponding formulas are awkward, and the contributions of these processes for the nanosystem under study are insignificant [14].

4. Analysis of the Results Obtained

We performed a specific calculation for a β -HgS nanofilm positioned into the external medium β -CdS. In this case, we used the following values of physical parameters [17] for such a system: $\Omega_{L0} = 27.8$ meV, $\Omega_{L1} = 57.2$ meV, $V = 1.35$ eV, $m_0 = 0.036$ and $m_1 = 0.2$ (in units of the mass of a free electron).

Each of the partial shifts of the main band bottom $\Delta_{\Lambda}(a, T)$ can be presented as the sum

$$\Delta_{\Lambda}(a, T) \approx \Delta_{\Lambda}^{(d)}(a, T) = \Delta_{\Lambda}(a, 0) + \Delta_{\Lambda}^{(+)}(a, T) + \Delta_{\Lambda}^{(-)}(a, T) \quad (28)$$

of contributions caused by the processes of interaction of an electron with virtual phonons at $T = 0$ K ($\Delta_{\Lambda}(a, 0)$) and real ones on their emission ($\Delta_{\Lambda}^{(+)}(a, T)$) and absorption ($\Delta_{\Lambda}^{(-)}(a, T)$) under the condition $T \neq 0$ K. This allows us to analyze the dependence of partial shifts of the main band bottom which are induced by various mechanisms of the electron-phonon interaction on the temperature and size of the nanosystem.

4.1. Interaction with bounded phonons

In Fig. 1, we give the plots of the temperature dependences of a partial shift of the main electron's energy band bottom caused by its interaction with bounded phonons of a nanofilm. Figure 1, *a* demonstrates the evolution of a partial shift $\Delta_{L0}^{(+)}(a, T)$ caused by the processes of emission of $L0$ -phonons for various values of the nanofilm thickness. As the temperature increases, its absolute value increases monotonically with the rate growing with the nanofilm thickness.

The temperature dependence of the component $\Delta_{L0}^{(-)}(a, T)$ shown in Fig. 1, *b* testifies that the processes related to the absorption of $L0$ -phonons also induce the increase in the absolute value of a shift of the main electron's energy band bottom with the temperature. However, the rate of this growth is a nonmonotonous function of the nanofilm thickness a . As the nanofilm thickness increase at a fixed temperature, the value of $\Delta_{L0}^{(-)}(a, T)$ firstly increases (curves 1–4) and then decreases (curves 5–10). The decrease in the absolute value of $\Delta_{L0}^{(-)}(a, T)$ begins, as a grows, at thicknesses greater than 30 β -HgS monolayers and is running nonmonotonously, which is illustrated by the position of curves 6–8.

The difference in the rates of variation of the components $\Delta_{L0}^{(\pm)}(a, T)$ with a change in the temperature

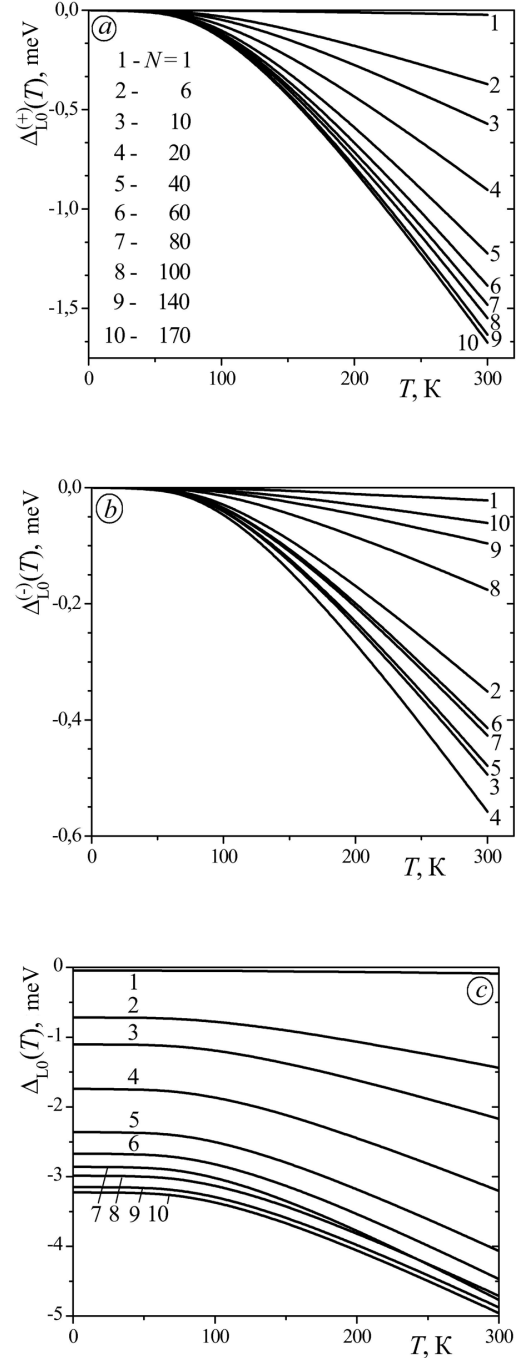


Fig. 1. Temperature dependences of partial shifts $\Delta_{L0}^{(-)}(a, T)$ (a), $\Delta_{L0}^{(+)}(a, T)$ (b), and $\Delta_{L0}(a, T)$ (c) in nanofilms with various numbers N of β -HgS nanolayers

at different nanofilm thicknesses is explained by the difference of the dependences of the functions $\Phi_{\lambda n}^{(\pm)}$ defining these rates on a (through the parameter N

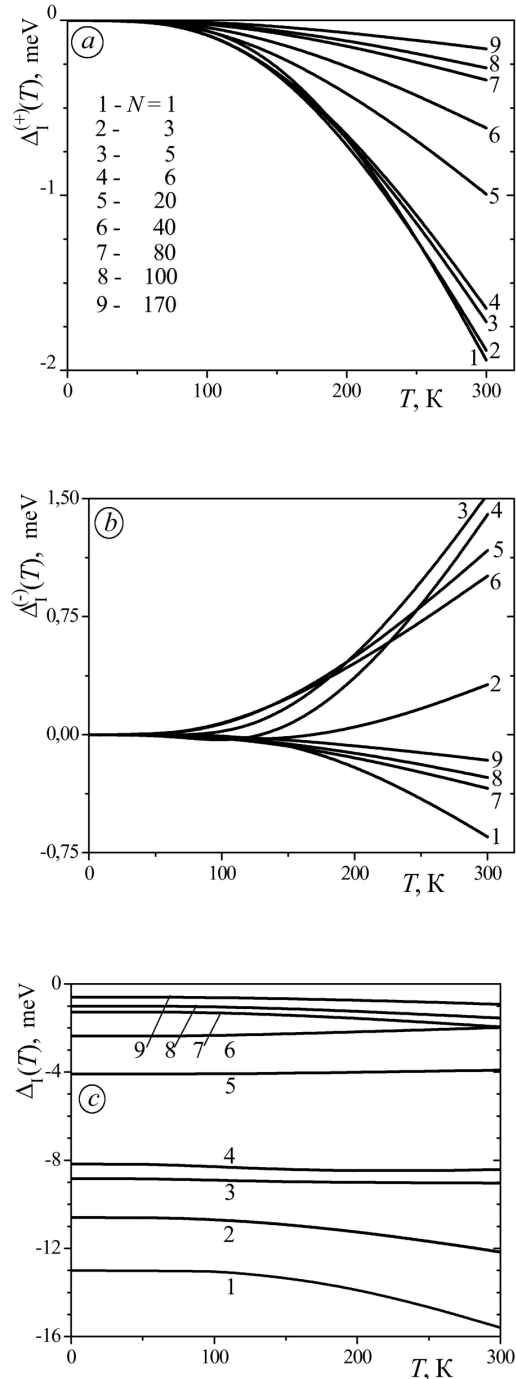


Fig. 2. Temperature dependences of partial shifts $\Delta_I^{(-)}(a, T)$ (a), $\Delta_I^{(+)}(a, T)$ (b), and $\Delta_I(a, T)$ (c) in nanofilms with various numbers N of β -HgS nanolayers

equal to the number of monolayers of β -HgS in the film). Since $\eta \gg 1$, the values of the functions in the numerator and denominator of formula (23) are positive

for small N . The change of their sign with increase in the nanofilm thickness happens practically at the same time moment, so that $\Phi_{L0}^{(+)}(a, T)$ is positive for any values of the parameters λ , n , and N , whereas the function $\Phi_{\lambda n}^{(-)}$ can take negative values at sufficiently large N under the condition $\xi_n < 1$. This condition is satisfied for levels, whose distance from the ground level is less than the energy of a bounded phonon Ω_{L0} . The number of such levels increases with the film thickness, which causes a decrease in the absolute value of $\Delta_{L0}^{(-)}(a, T)$. The nonmonotonicity of its dependence on a can be explained by the fact that, as the film thickness increases, values of the energies of all levels decrease. Therefore, the condition $\xi_n < 1$ for films with close thicknesses corresponds to different numbers of levels which give, moreover, different contributions to the quantity $\Delta_{L0}^{(-)}(a, T)$.

For any thicknesses and temperatures of a nanofilm, $|\Delta_{L0}^{(-)}(a, T)| < |\Delta_{L0}^{(+)}(a, T)|$, and the contribution of continual states is insignificant. Therefore, the absolute value of the total $L0$ -phonon shift of the electron's band bottom $\Delta_{L0}(a, T)$ turns out to be an increasing function of the temperature (Fig. 1, c). The temperature changes of the partial contribution of the electron-phonon interaction with bounded phonons become significant at temperatures higher than 100 K for films with any thickness, except for very thin films (curve 1). In the last case, the temperature effect can be neglected due to the smallness of all three terms on the right-hand side of (28).

4.2. Interaction with interface phonons

The thermal genesis of a partial shift of the main band bottom $\Delta_I(a, T)$ and its components $\Delta_I^{(\pm)}(a, T)$ caused by the interaction of an electron with interface phonons in nanofilms with various thicknesses a is shown in Fig. 2. It is seen that the character of the thermal genesis of $\Delta_I(a, T)$ is more complicated than that in the case of the interaction with bounded phonons.

The increase of the temperature leads to an increase of the shift related to the emission of interface phonons (Fig. 2, a). But, as distinct from the interaction with $L0$ -phonons, the growth rate of $\Delta_I^{(+)}(a, T)$ decreases rapidly with increase in the nanofilm thickness.

The shift $\Delta_I^{(-)}(a, T)$ caused by the interaction of an electron with interface phonons in the processes of their absorption has a nonmonotonous dependence on both the temperature and the film thickness (Fig. 2, b). The reason for such complicated behavior of $\Delta_I^{(-)}(a, T)$

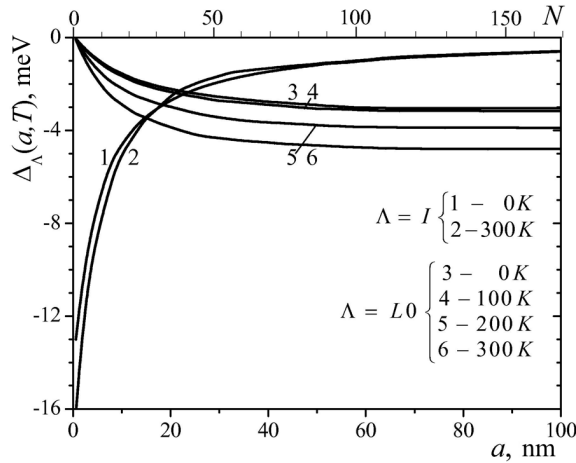


Fig. 3. Partial shifts $\Delta_{L0,I}(a, T)$ versus the nanofilm thickness a at various temperatures T

consists in that the numerator of the integrand of the second term in formula (25) is positive and decreases with increase in $q_{||}$, and the denominator increases, by changing the sign on the passage through the discontinuity point. The positions of the discontinuity points (they are different for low- and high-energy phonons) are determined by a nanofilm thickness, and they shift to the region of greater values of $q_{||}$ with increase in a . For this reason, the integral which is calculated in the sense of the principal value takes values differing from one another by their signs and moduli, which leads to the difference of the temperature genesis of the shifts $\Delta_I^{(-)}(a, T)$ and, therefore, $\Delta_I(a, T)$ in films of various thicknesses (Fig. 2,c).

In Fig. 3, we show the dependences of partial shifts $\Delta_I(a, T)$ (curves 1-2) and $\Delta_{L0}(a, T)$ (curves 3-6) on the nanofilm thickness. It is seen that the contribution of interface phonons is dominant in very thin nanofilms, and the contribution of bounded ones prevails in thick nanofilms. The interaction of an electron with both branches of phonons induces the increase of the shift of the main band bottom to the region of lower energies as the temperature grows. But such an increase is essential only at temperatures higher than 100 K.

The dependences of the total shift $\Delta(a, T)$ of the main electron's band bottom on the nanofilm thickness a at fixed temperatures and on the temperature T at fixed thicknesses a are presented in Figs. 4 and 5, respectively. It is seen from both figures that, irrespective of the nanofilm thickness, the band bottom shifts slightly (by several meV) to the region of lower energies as the temperature grows.

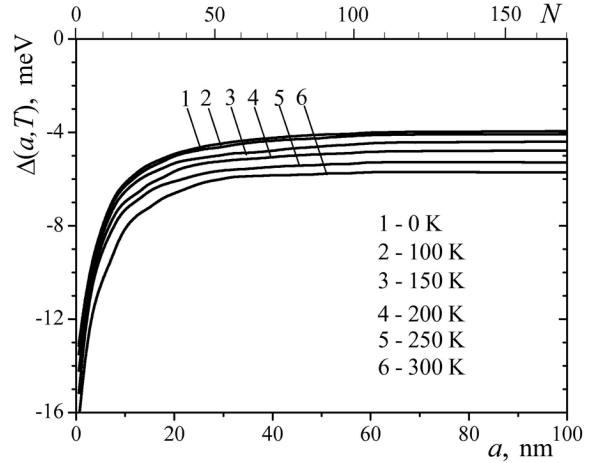


Fig. 4. Total shift $\Delta(a, T)$ versus the nanofilm thickness a at various temperatures T

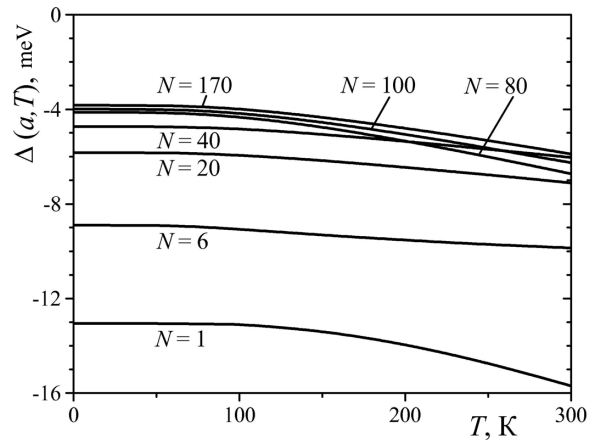


Fig. 5. Total shift $\Delta(a, T)$ versus the temperature T in nanofilms with various numbers N of β -HgS nanolayers

Taking into account that the used model of effective mass and rectangular potential barrier works satisfactorily for nanofilms, whose thickness exceeds several monolayers of β -HgS, we may draw the following general conclusion. The interaction of electrons with interface phonons forms the temperature shift of the main electron's band bottom in superthin films ($N < 10$). In thin films ($10 \leq N \leq 100$), the contributions of I - and $L0$ -phonons to the temperature shift are almost identical. In thick films ($N > 100$), the shift is mainly formed by $L0$ -phonons and asymptotically approaches the value characteristic of a massive β -HgS crystal, which is clear from the physical reasoning.

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ТЕМПЕРАТУРНИЙ ГЕНЕЗИС ДНА ОСНОВНОЇ ЗОНИ ЕНЕРГІЙ ЕЛЕКТРОНА У ПЛОСКІЙ НАНОПЛІВЦІ

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Резюме

У наближенні діелектричного континууму для фононів та прямокутних потенціалів і ефективних мас – для електронів, методом функцій Гріна виконано аналітичний розрахунок перенормованого фононами положення дна основної електронної зони у плоскій квантовій ямі – напівпровідниковій наноплівці, вміщеній у зовнішнє напівпровідникове середовище. На прикладі плоскої наногетеросистеми β -HgS/ β -CdS виконано числовий розрахунок зміщення дна зони електрона як функції товщини плівки і температури. Показано, що зі збільшенням температури електрон-фононна взаємодія у процесах поглинання і випромінювання приводить до зміщення дна зони в діапазон менших енергій. Встановлено механізми температурного збільшення зсуву у плівках різної товщини та причини різних швидкостей температурних зміщень дна електронної зони.