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Presurface Exciton Spectrum at Finite Temperatures

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The Hamiltonian of the presurface excitons interacting with the bulk and interface phonons in a heterosystem with a plane interface is obtained in the representation of second quantization in all variables. The spectrum parameters (shift and half-width) of the shape function of the basic band at arbitrary temperatures are calculated with the help of the Green function method. The temperature dependence of the spectrum parameters is studied and the physical mechanism of their formation is established on the example of particular heterosystems.

В представлении вторичного квантования по всем переменным системы найден гамильтониан приповерхностных экситонов, взаимодействующих с объёмными и поверхностными фононами в гетеросистеме с плоской границей раздела сред. Методом функций Грина рассчитаны спектральные параметры (сдвиг и полуширина) функции формы основной полосы приповерхностного экситона при произвольных температурах. Получена температурная зависимость спектральных параметров и установлен физический механизм их формирования на примере конкретных гетеросистем.

1. Introduction

The particular interest in the investigation of spatially confined and heterogeneous systems [1 to 7] is due to a number of reasons in the recent years. First, the highly developed technology used in producing semiconductors, gives an opportunity to create perfect heterosystems; second, the evidence of effects which are not characteristic of ordinary systems makes this use very various. A successful application of these systems is only possible if there is complete information about the processes taking place in them. No doubt, the spectrum parameters of quasiparticles in such systems are very important. The presence of surfaces or interfaces with different dielectric constants gives rise to the creation of different types of excitons. It is clear that the spectrum in homogeneous and heterogeneous systems can essentially differ because besides the electron–hole interaction some other factors appear (size quantization, interaction with image charges, etc.). Then, in bulk homogeneous semiconductors besides the kinetic energy the basic and principal energy is that of electron–hole interaction causing the creation of Wannier-Mott excitons [8]. In a double heterosystem with small quantum well thickness the energy of size quantization correlates with the energy of electron–hole interaction, but the energy of an electron and a hole interacting with their images does not play a fundamental role in the formation of the exciton spectrum, as is shown in [9]. In a single heterostructure the size quantization is absent and therefore at definite conditions the interaction of electrons and holes with their

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images can cause the exciton localization near the contacting medium surfaces, consequently, the presurface exciton (PE) is created.

The interaction with phonons influences the spectrum of any quasiparticles in semiconductor systems due to virtual vibrations even at $T = 0$ K. The temperature dependence of the spectrum is fully determined by phonons when the concentration of the quasiparticles is small in systems without any impurities. Therefore, the exciton–phonon interaction is to be taken into account in the basic model of the system. The phonon spectrum in heterostructures essentially differs from the spectrum in homogeneous crystals, e.g. in [10, 11] it was shown that in heterosystems the longitudinally polarized phonons were modified and new interface phonons arose. It was also shown that both types of phonons interact with charge carriers. The influence of the electron–phonon interaction on the different physical characteristics was later studied in [12 to 14].

The PE properties were investigated by a number of authors on the basis of different models with and without phonons. However, in most cases the Schrödinger problem was not solved self-consistently but in significant approximations. For example, in [15, 16] it was assumed that the electron was bound on the interface or on an arbitrarily fixed distance from it. The PE self-consistent model localized by electrostatic image forces near the surface of the heterosystem was suggested in [17]. There the Schrödinger equation was solved with the help of a combined approach of perturbation theory and a variational method with parameters included into the system Hamiltonian (see also the theory of atomic spectra in [20]). This gave an opportunity to obtain the quantum wave functions and the energy spectrum of PE without consideration of quasiparticle interactions with polarized phonons. In [18, 19] the theory of PE spectra near the interface was developed taking into account the polarized phonons at $T = 0$ K. A model was used where the electron and hole of an exciton interacted much stronger with phonons than between each other. The temperature dependence of the PE spectrum parameters was not researched in those papers.

The present paper proposes one of the possible variations of formulating a self-consistent theory of the interaction of the PE and polarization vibrations of the heterosystem with a plane interface. The Hamiltonian of the exciton–phonon system in the representation of occupation numbers on all variables is obtained. In the one-phonon approximation the shape function of the basic zone is calculated and analyzed with the help of the Green function method. The temperature dependence of the shift and half-width of the shape function of the PE basic band is discovered on the example of the analysis of a particular heterosystem.

2. Hamiltonian of Presurface Exciton Interacting with Inertial and Uninertial Polarization of a Single Heterosystem

The following model of PE is investigated. An electron (r_e, m_e) and a hole (r_h, m_h) are in a medium with dielectric constant ε_1 in contact with a medium having the dielectric constant ε_2. These media have a plane interface. The Cartesian coordinate system is chosen in such a way that the XOY plane coincides with the crystal interface, and the OZ axis is directed into the exciton-containing medium (Fig. 1). There are two types of polarizations in such a system: the inertial type caused by the polarized phonons and the uninertial one caused by the difference of the dielectric constants of the contacting media (equivalent to the appearance of the image electrostatic charges in the system). Thus, an electron (e) and a hole (h) interact (i) with each other; with their "own" and "strange" electrostatic images (uninertial polarization), and (ii) with the polarized phonons (inertial polarization).

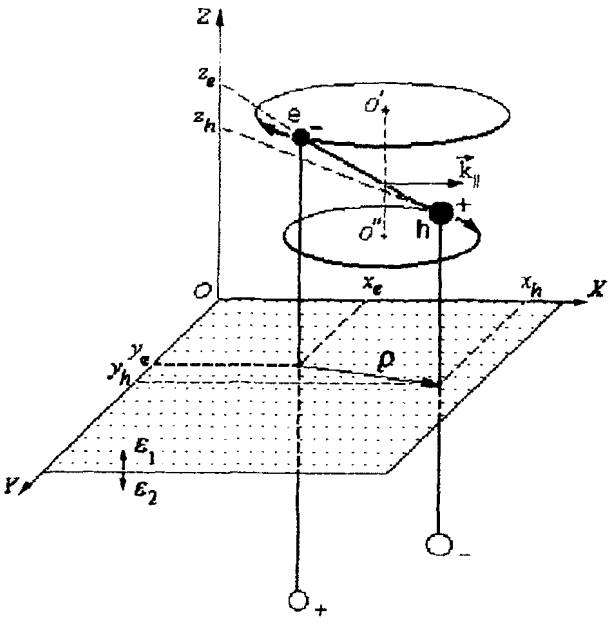

Fig. 1. Model of the presurface exciton

The total Hamiltonian of the system has the form

$$H = H_{ex} + H_{ph} + H_{ex-ph}. \tag{1}$$

Here

$$H_{ex} = -\frac{\hbar^2\nabla_e^2}{2m_e} - \frac{\hbar^2\nabla_h^2}{2m_h} - \frac{e^2}{\varepsilon_1 r_{ex}} - \frac{\gamma e^2}{\varepsilon_1 z_e} - \frac{\gamma e^2}{\varepsilon_1 z_h} + \frac{4\gamma e^2}{\varepsilon_1\sqrt{\varrho^2 + (z_e + z_h)^2}}, \tag{2}$$

where the first two terms describe the kinetic energy of electron and hole, respectively; the third term represents the potential energy of electron–hole interaction; the fourth (fifth) term represent the potential energies of the electron (hole) interacting with their "own" images; and the last one is the energy of electron and hole interacting with "strange" images; $\gamma = (\varepsilon_2 - \varepsilon_1)/4(\varepsilon_2 + \varepsilon_1)$. We assume that $\varepsilon_2 > \varepsilon_1$, then as it is shown in [17], the electron and hole are bound with their electrostatic images in the PE near the media interface (Fig. 1).

The Schrödinger equation

$$H_{ex}\,|f, \boldsymbol{k}_\parallel\rangle = E_f(\boldsymbol{k}_\parallel)\,|f, \boldsymbol{k}_\parallel\rangle \tag{3}$$

was solved in [17]. It was established that the PE energy spectrum

$$E_f(\boldsymbol{k}_\parallel) = E_f + \frac{\hbar^2\boldsymbol{k}_\parallel^2}{2m_{ex}}; \qquad (m_{ex} = m_e + m_h) \tag{4}$$

was characterized by both a total set of four quantum numbers $f = \{n, m, n_e, n_h\}$, where $n = 0, 1, 2, \ldots, \infty$; $m = 0, \pm 1, \pm 2, \ldots, \pm n$ are the basic and magnetic quantum numbers of the "plane" subsystem; $n_e, n_h = 1, 2, \ldots, \infty$ are the basic quantum numbers of the "vertical" subsystem; and by the two-dimensional wave vector $\boldsymbol{k}_\parallel$ describing the transitional movement of PE as a whole in the plane parallel to the medium interface. The PE energy

levels are defined by formula (19) in [17]. The wave functions are given by the following expressions:

$$|f, \boldsymbol{k}_{\|}\rangle = \exp\left[i \frac{\boldsymbol{k}_{\|}}{2} \left(\boldsymbol{r}_{e\|} + \boldsymbol{r}_{h\|} + \boldsymbol{\varrho} \frac{m_e - m_h}{m_{ex}} \right) \right] \Phi^0_{nm}(\boldsymbol{\varrho})\, \Psi^0_{n_e}(z_e)\, \Psi^0_{n_h}(z_h)\,, \tag{5}$$

where

$$\Phi^0_{nm}(\varrho) = \left[\frac{(n - |m|)!}{\pi a^2_{\|n} (n + \frac{1}{2})^3 [(n + |m|)!]^3} \right]^{1/2} \exp\left[- \frac{\varrho}{a_{\|n}(n + \frac{1}{2})} + im\varphi \right] \times \left(\frac{2\varrho}{a_{\|n}(n + \frac{1}{2})} \right)^{|m|} \mathrm{L}^{2|m|}_{n+|m|} \left(\frac{2\varrho}{a_{\|n}(n + \frac{1}{2})} \right), \tag{6}$$

$$\Psi^0_{\perp n_j}(z_j) = \frac{z_j}{\sqrt{2n_j}} \left(\frac{2}{n_j a_{\perp n_j}} \right)^{3/2} \exp\left(-z_j / n_j a_{\perp n_j}\right) \mathrm{F}\left(1 - n_j, 2, \frac{2z_j}{n_j a_{\perp n_j}} \right). \tag{7}$$

Here we use the evident notation described in [17] in details. Introducing the quantized wave function

$$\hat{\Psi} = \sum_{f, \boldsymbol{k}_{\|}} |f, \boldsymbol{k}_{\|}\rangle\, \hat{a}_{f, k_{\|}}\,, \tag{8}$$

according to the general rules [21] the Hamiltonian of the PE (taking into account the uninertial medium polarization) is obtained in the representation of second quantization,

$$H_{ex} = \sum_{f, \boldsymbol{k}_{\|}} E_{f, \boldsymbol{k}_{\|}} \hat{a}^+_f(\boldsymbol{k}_{\|})\, \hat{a}_f(\boldsymbol{k}_{\|})\,, \tag{9}$$

where $\hat{a}^+_f(\boldsymbol{k}_{\|})$, $\hat{a}_f(\boldsymbol{k}_{\|})$ are the operators of the exciton state f (with two-dimensional quasi-momentum $\boldsymbol{k}_{\|}$) creation and annihilation of boson type.

The second term in (1) is H_{ph}, i.e. the Hamiltonian of the polarization vibrations of the heterosystem under study in the present paper. The phonon spectrum was examined and obtained in papers of different authors [10 to 13] with the help of the continuum model. In the representation of second quantization on the phonon variables we have

$$H_{ph} = \sum_{\lambda=1}^{4} \sum_{\boldsymbol{q}_{\|}, q_z} \Omega_\lambda [\hat{b}^+_{\lambda, q_z}(\boldsymbol{q}_{\|})\, \hat{b}_{\lambda, q_z}(\boldsymbol{q}_{\|}) + \tfrac{1}{2}]\,;$$
$$\lambda = 1, 2, 3, 4 = \mathrm{s}, \mathrm{a}, \mathrm{L}, \mathrm{T}\,, \qquad q_z = 0\,, \quad \text{when} \quad \lambda = 1, 2 = \mathrm{s}, \mathrm{a}\,, \tag{10}$$

where $\hat{b}^+_{\lambda, q_z}(\boldsymbol{q}_{\|})$, $\hat{b}_{\lambda, q_z}(\boldsymbol{q}_{\|})$ are the operators of the phonon state creation and annihilation of boson type; $\Omega_{\mathrm{L}, n}$, $\Omega_{\mathrm{T}, n}$ are the energies of the longitudinal and transverse optical vibrations of the n-th medium; Ω_s, Ω_a are the energies of the symmetrical (s) and antisymmetrical (a) interface vibrations defined by the solutions of the dispersion equation

$$\sum_{n=1}^{2} \varepsilon_{\infty, n} \frac{\Omega^2 - \Omega^2_{\mathrm{L}, n}}{\Omega^2 - \Omega^2_{\mathrm{T}, n}} = 0\,, \tag{11}$$

where $\varepsilon_{\infty, n}$ is the high frequency dielectric constant of the n-th medium.

The third term in (1) is H_{ex-ph}, i.e. the Hamiltonian of the exciton–phonon interaction obtained according to the general theory [20] of the transition to the representation of second quantization,

$$H_{ex-ph} = \int \Psi^+(\boldsymbol{r}_e, \boldsymbol{r}_h) [H_{e-ph} + H_{h-ph}]\, \Psi(\boldsymbol{r}_e, \boldsymbol{r}_h)\, \mathrm{d}^3 \boldsymbol{r}_e\, \mathrm{d}^3 \boldsymbol{r}_h\,, \tag{12}$$

where the interaction Hamiltonians of either the electron (H_{e-ph}) or the hole (H_{h-ph}) with the phonons of the heterosystem are found already in the mixed representation in [11, 12, 14],

$$H_{e,h-ph} = \sum_{\lambda=1}^{4} \sum_{\boldsymbol{q}_\parallel, q_z > 0} C_\lambda(\boldsymbol{q}_\parallel, q_z) \exp(i\boldsymbol{q}_\parallel \boldsymbol{r}_{\parallel(e,h)}) D_\lambda(z_{e,h}) [\hat{b}_{\lambda,q_z}(\boldsymbol{q}_\parallel) + \hat{b}^+_{\lambda,q_z}(-\boldsymbol{q}_\parallel)], \tag{13}$$

where

$$C^{e,h}_{\lambda=1,2} = \sqrt{\frac{4\pi e^2 \Omega_\lambda}{d^2\boldsymbol{q}_\parallel [\beta_1^{-1}(\Omega_\lambda) + \beta_2^{-1}(\Omega_\lambda)]}} \exp(-q_z |z_{e,h}|),$$

$$C^{e,h}_{\lambda=3} = \sqrt{\frac{2\pi e^2 \Omega_L(\varepsilon_\infty^{-1} - \varepsilon_0^{-1})}{d^3(\boldsymbol{q}_\parallel^2 + q_z^2)}} \theta(z_{e,h}) \sin(q_z z_{e,h}),$$

$$D_{\lambda=1,2}(z_{e,h}) = \exp(-q_z |z_{e,h}|),$$

$$D_{\lambda=3}(z_{e,h}) = \theta(z_{e,h}) \sin(q_z z_{e,h}),$$

$$\beta_n(\Omega_\lambda) = (\varepsilon_{\infty,n}^{-1} - \varepsilon_{0,n}^{-1}) \frac{\Omega^2_{L,n}}{\Omega^2_\lambda} \left(\frac{\Omega^2_\lambda - \Omega^2_{T,n}}{\Omega^2_{L,n} - \Omega^2_{T,n}} \right),$$

$\varepsilon_{0,n}$ is the low frequency dielectric constant of the n-th medium, d is the length of the basic region of the system, θ is the theta-function, and $C_4 \equiv 0$ because the charged quasiparticles do not interact with the transverse phonons [11, 12].

After some corresponding transformations one can obtain the Hamiltonian of the exciton–phonon interaction in the representation of second quantization on all variables of the system from (12)

$$H_{ex-ph} = \sum_{\substack{\lambda, f_1, f_2 \\ \boldsymbol{k}_\parallel, \boldsymbol{q}_\parallel, q_z > 0}} F_{\lambda, f_1, f_2}(\boldsymbol{q}_\parallel, q_z) \hat{a}^+_{f_1}(\boldsymbol{k}_\parallel + \boldsymbol{q}_\parallel) \hat{a}_{f_2}(\boldsymbol{k}_\parallel) [\hat{b}_{\lambda,q_z}(\boldsymbol{q}_\parallel) + \hat{b}^+_{\lambda,q_z}(-\boldsymbol{q}_\parallel)]. \tag{14}$$

Here $f = n, n_e, n_h, m$; $n = 0, 1, 2, \ldots \infty$; $n_e, n_h = 1, 2, 3, \ldots \infty$; $m = 0, \pm 1, \pm 2, \ldots \pm n$, and the exciton–phonon binding functions $F_{\lambda,f_1,f_2}(\boldsymbol{q}_\parallel, q_z)$ are given by the following expression:

$$\begin{aligned} F_{\lambda,f_1,f_2}(\boldsymbol{q}_\parallel, q_z) = C_\lambda \iint \mathrm{d}^2\boldsymbol{\varrho} \exp\left(i\boldsymbol{q}_\parallel \boldsymbol{\varrho}_\parallel \frac{\alpha_1 - \alpha_2}{2} \right) \Phi^+_{n_1,m_1}(\varrho) \Phi_{n_2,m_2}(\varrho) \\ \times \int_0^\infty \Psi^+_{n_{1e}}(z_e) \Psi_{n_{2e}}(z_e) \, \mathrm{d}z_e \\ \times \int_0^\infty \Psi^+_{n_{1h}}(z_h) \Psi^+_{n_{2h}}(z_h) [D_\lambda(z_e) - D_\lambda(z_h)] \, \mathrm{d}z_h, \end{aligned} \tag{15}$$

where the wave functions $\Phi_{n,m}(\varrho)$, $\Psi_{n_e}(z_e)$, $\Psi_{n_h}(z_h)$ are given by (6), (7).

However, the Hamiltonian (14) obtained in such a way is general but rather complicated. In the present paper only heterosystems where the PE basic level (zone) is located far

enough from other levels will be considered further on. Therefore, neglecting the interaction between zones (with different f) due to the phonons, one can obtain a comparatively simple interaction Hamiltonian,

$$H_{\mathrm{ex-ph}} = \sum_{\substack{\lambda, q_z > 0 \\ \boldsymbol{k}_\parallel, \boldsymbol{q}_\parallel}} F_\lambda(\boldsymbol{q}_\parallel, q_z)\, \hat{a}^+(\boldsymbol{k}_\parallel + \boldsymbol{q}_\parallel)\, \hat{a}(\boldsymbol{k}_\parallel)\, [\hat{b}_{\lambda, q_z}(\boldsymbol{q}_\parallel) + \hat{b}^+_{\lambda, q_z}(-\boldsymbol{q}_\parallel)]\,. \tag{16}$$

Here $\hat{a}_0 = \hat{a}$, $\hat{a}_0^+ = \hat{a}^+$ are introduced and according to (15) the binding functions with the presurface phonons are

$$F_{\lambda=1,2}(\boldsymbol{q}_\parallel, q_z) = \sqrt{\frac{2e^2 a \Omega_\lambda}{d^2 Q_\parallel [\beta_1^{-1}(\Omega_\lambda) + \beta_2^{-1}(\Omega_\lambda)]}}\; \zeta_{\lambda=1,2}(Q_\parallel)\,, \tag{17}$$

where

$$\zeta_{\lambda=1,2}(Q_\parallel) = \sum_{p=1}^{2} \frac{(-1)^p}{(1 + \alpha_p Q_\parallel^2)^{3/2}\,(1 + \gamma_p Q_\parallel)^3}\,,$$

and the binding function with half-bulk phonons is

$$F_{\lambda=3}(\boldsymbol{q}_\parallel, q_z) = \sqrt{\frac{8e^2 a \Omega_{\mathrm{L}} (\varepsilon_\infty^{-1} - \varepsilon_0^{-1})}{\pi d^3 (Q_\parallel^2 + Q_z^2)}}\; \zeta_{\lambda=3}(\boldsymbol{Q}_\parallel, Q_z)\,, \tag{18}$$

where

$$\zeta_{\lambda=3}(\boldsymbol{Q}_\parallel, Q_z) = \sum_{p=1}^{2} \frac{(-1)^p\, \gamma_p Q_z (3 - \gamma_p^2 Q_z^2)}{(1 + \alpha_p Q_\parallel^2)^{3/2}\,(1 + \gamma_p^2 Q_z^2)^3}\,.$$

The values

$$\alpha_p = \frac{\pi^2 a_\parallel^2 m_{\parallel p}^2}{16 a^2 m_\parallel^2}\,, \qquad \gamma_p = \frac{\pi a_{\perp p}}{2a}$$

are connected with the corresponding effective Bohr radii of the "plane" ($a_\parallel$) and "vertical" ($a_{\perp \mathrm{e}}$, $a_{\perp \mathrm{h}}$) exciton terms introduced in [17], where a is the lattice constant and $\boldsymbol{Q} = a\boldsymbol{q}/\pi$ a dimensionless wave vector.

3. Exciton Band Shape Function and PE Basic Zone Renormalization

We examine a simplified model of the PE which is located in the basic zone and interacts with phonons in a single heterosystem in such a way that the transitions into other zones can be neglected. This exciton is characterized by the energy E_0 of the zone bottom (it includes the energy of its internal movement, the energy of the interaction between an electron and a hole as well as with their images), and the plane quasi-momentum $\boldsymbol{k}_\parallel$.

According to the general theory [21] the retarded Green function is used to study the PE spectral characteristics

$$G(\boldsymbol{k}_\parallel, t) = -i\theta(t)\, \langle [\hat{a}(\boldsymbol{k}_\parallel, t),\, \hat{a}^+(\boldsymbol{k}_\parallel, 0)] \rangle\,. \tag{19}$$

Its Fourier image is connected (at $\boldsymbol{k}_{\parallel} = 0$) with a shape function by the relation

$$\pounds(\omega) = -\operatorname{Im} G(\omega), \tag{20}$$

where $G(\omega)$ is defined from the Dyson equation

$$G(\omega') = \{\omega' - E_0 - M(\omega')\}^{-1} \qquad (\omega' = \omega + i\varepsilon, \varepsilon \to +0), \tag{21}$$

in terms of the mass operator (MO) $M(\omega')$. In case of a small exciton concentration the total MO is defined by an infinite set of respective Feynman diagrams [22] or by an infinite integral branching fraction [23] taking into account many-phonon processes. However, as we are going to study only the energy region near the bottom of the exciton zone (without taking into account the bound and free exciton–phonon states) and heterosystems with weak binding,

$$\mu = \sum_{\lambda, \boldsymbol{q}_{\parallel}, q_z > 0} \frac{|F_\lambda(\boldsymbol{q}_{\parallel}, q_z)|^2}{\Omega_\lambda^2} < 1, \tag{22}$$

when calculating the MO one can examine the one-phonon approximation

$$M(\omega') = \sum_{\lambda} M_\lambda(\omega') = \sum_{\lambda, \boldsymbol{q}_{\parallel}, q_z > 0} |F_\lambda(q_{\parallel}, q_z)|^2 \times \left[\frac{1 + \nu_\lambda}{\hbar\omega' - E_0 - \dfrac{\hbar^2 q_{\parallel}^2}{2m_{\parallel}} - \Omega_\lambda} + \frac{\nu_\lambda}{\hbar\omega' - E_0 - \dfrac{\hbar^2 q_{\parallel}^2}{2m_{\parallel}} + \Omega_\lambda} \right], \tag{23}$$

where $\nu_\lambda = \{\exp(\Omega_\lambda q/kT) - 1\}^{-1}$ is the average value of the occupation numbers of the λ-mode phonons.

The analysis and calculations are conveniently performed with dimensionless parameters,

$$\tilde{\Omega}_\lambda = \frac{\Omega_\lambda}{\Omega_{\min}}, \qquad \xi = \frac{\hbar\omega' - E_0}{\Omega_{\min}}, \qquad \eta = \frac{\hbar^2\pi^2}{2m_{\parallel} a^2 \Omega_{\min}},$$

$$\Omega_{\min} = \min\{\Omega_s, \Omega_a, \Omega_L\}.$$

Then, changing summation into integration over the dimensionless wave vectors in the cylinder coordinate system for the dimensionless MO one can get the equation

$$\mathrm{m}(\xi) = \sum_{\lambda = s,a,L} \mathrm{m}_\lambda(\xi) = \Omega_{\min}^{-1} \sum_{\lambda = s,a,L} M_\lambda(\omega'), \tag{24}$$

where

$$\mathrm{m}_{s,a}(\xi) = \frac{\pi e^2 \Omega_{s,a}}{a\Omega_{\min}^2} \frac{1}{\beta_1^{-1}(\Omega_{s,a}) + \beta_2^{-1}(\Omega_{s,a})} \int_0^{\infty} \zeta_{s,a}^2(\boldsymbol{Q}_{\parallel}) \times \left\{ \frac{1 + \nu_{s,a}}{\xi - \eta Q_{\parallel}^2 - \tilde{\Omega}_{s,a}} + \frac{\nu_{s,a}}{\xi - \eta Q_{\parallel}^2 + \tilde{\Omega}_{s,a}} \right\} \mathrm{d}Q_{\parallel} \tag{25}$$

are terms describing the interaction between the PE and interface s- and a-modes;

$$\mathfrak{m}_{\mathrm{L}}(\xi) = \frac{2e^2\Omega_{\mathrm{L}}}{a\Omega_{\min}^2}\left(\frac{1}{\varepsilon_{\infty,1}} - \frac{1}{\varepsilon_{0,1}}\right)\int_0^\infty \left\{\frac{1+\nu_{\mathrm{L}}}{\xi - \eta Q_\parallel^2 - \tilde{\Omega}_{\mathrm{L}}} + \frac{\nu_{\mathrm{L}}}{\xi - \eta Q_\parallel^2 + \tilde{\Omega}_{\mathrm{L}}}\right\} \mathrm{d}Q_\parallel$$

$$\times \int_0^\infty \zeta_{\mathrm{L}}^2(Q_\parallel, Q_z)\frac{Q_\parallel}{Q_\parallel^2 + Q_z^2}\,\mathrm{d}Q_z \tag{26}$$

is a term describing the interaction between the exciton and half-bulk LO-phonons.

A further calculation of $\mathrm{Re}\,\mathfrak{m}(\xi)$ and $\mathrm{Im}\,\mathfrak{m}(\xi)$ in the actual region $\xi < 0$ is performed according to (17) with the help of the Dirac equality $1/(x + i\varepsilon) \equiv P(1/x) - i\pi\,\delta(x)$. Therefore, in $\mathrm{Re}\,\mathfrak{m}(\xi)$ there are the same integrals as in $\mathfrak{m}(\xi)$, but in the terms containing poles the respective integrals are examined in the sense of the principle value and numerically calculated due to the fact that the parameter ξ is real. In the mentioned energy region the first terms in the MO (17) do not contain poles while others do. Therefore $\mathrm{Im}\,\mathfrak{m}(\xi \leqq 0)$ is calculated with the help of the corresponding Dirac δ-functions and it is given by the following analytical expressions:

$$\mathrm{Im}\,\mathfrak{m}_{\mathrm{s,a}}(\xi \leqq 0) = -\frac{\pi^2 e^2 \Omega_{\mathrm{s,a}}}{2a\Omega_{\min}^2}\frac{1}{\beta_1^{-1}(\Omega_{\mathrm{s,a}}) + \beta_2^{-1}(\Omega_{\mathrm{s,a}})}\frac{\theta(\xi + \Omega_{\mathrm{s,a}})}{\sqrt{\eta(\xi + \Omega_{\mathrm{s,a}})}}$$

$$\times \left[\sum_{p=1}^{2}\frac{(-1)^p}{\left(1 + \dfrac{\alpha_p(\xi + \Omega_{\mathrm{s,a}})}{\eta}\right)^{3/2}\left(1 + \gamma_p\sqrt{\dfrac{\xi + \Omega_{\mathrm{s,a}}}{\eta}}\right)}\right]^2 \nu_{\mathrm{s,a}}, \tag{27}$$

$$\mathrm{Im}\,\mathfrak{m}_{\mathrm{L}}(\xi \leqq 0) = -\frac{\pi e^2 \Omega_{\mathrm{L}}}{a\Omega_{\min}^2}\left(\frac{1}{\varepsilon_{\infty,1}} - \frac{1}{\varepsilon_{0,1}}\right)\theta(\xi + \Omega_{\mathrm{L}})\sqrt{\frac{\xi + \Omega_{\mathrm{L}}}{\eta^3}}$$

$$\times \int_0^1 \mathrm{d}x \left[\sum_{p=1}^{2}\frac{(-1)^p \gamma_p x\left[3 - \gamma_p^2\dfrac{\xi + \Omega_{\mathrm{L}}}{\eta}x^2\right]}{\left(1 + \alpha_p\dfrac{\xi + \Omega_{\mathrm{L}}}{\eta}(1 - x^2)\right)^{3/2}\left(1 + \gamma_p^2\dfrac{\xi + \Omega_{\mathrm{L}}}{\eta}x^2\right)^3}\right]^2 \nu_{\mathrm{L}}. \tag{28}$$

A further calculation is performed at fixed parameters of the heterosystem.

4. Discussion

For the comparison of the PE spectra with their analogues in bulk crystals we have examined the PE in the Cu_2O/TlBr and $Cu_2O/SrTiO_3$ heterosystems. The parameters of these systems are given in Table 1. We have chosen these crystals due to the following considerations. Their dielectric constants are bigger than that of Cu_2O. Thus, the forces of the electron and hole interaction with their image charges bind an electron and a hole near the interface between Cu_2O and the medium, consequently, creating a PE. The

Table 1
Parameters of the Cu_2O/TlBr and $Cu_2O/SrTiO_3$ heterosystems

	ε_0	ε_∞	m_e/m_0	m_h/m_0	Ω_T (cm^{-1})	Ω_L (cm^{-1})	Ω_s (cm^{-1})	Ω_a (cm^{-1})
Cu_2O	9	4.2	0.3	1.4	170.8	250	–	–
TlBr	29.8	5.42	–	–	49.5	116	215	79
$SrTiO_3$	320	5	–	–	15.4	123.2	218	72

parameters which characterize the exciton–phonon binding forces in these systems are the following:

$$\mu_{Cu_2O/TlBr} = 0.68 < 1\,, \qquad \mu_{Cu_2O/SrTiO_3} = 0.79 < 1\,.$$

We suppose that the one-phonon approximation of the MO is sufficient for the analysis of the £ shape function and its spectral parameters $\Delta(T)$, $\Gamma(T)$.

According to the general theory [21], the total shift of the maximum of the £ function is defined as

$$\Delta(T) = \Delta_0 + \Delta_T = \Omega_{min}\,\mathrm{Re}\,\mathfrak{M}(\xi = \xi_0)\,, \tag{29}$$

where ξ_0 is obtained from the solution of the dispersion equation $\xi = \mathrm{Re}\,\mathfrak{M}(\xi)$. Here Δ_0 is independent of the temperature (it does not contain v_λ) term of the real part of the MO (24). It forms the shift of the PE zone bottom due to the radiation of virtual phonons; Δ_T depends on the temperature (throughout v_λ) term of the real part of the MO (24) forming the temperature dependence of the PE zone bottom in the energy scale due to the PE interaction with real phonons during their creation and annihilation processes.

The half-width

$$\Gamma(T) = \Gamma_T = -\Omega_{min}\,\mathrm{Im}\,\mathfrak{M}(\xi = \xi_0) \tag{30}$$

is defined according to (27), (28) only by annihilation processes of real phonons.

Fig. 2a, b show the result of £(ξ) calculation for both heterosystems and its temperature dependence. It is clear that for both systems the temperature dependence of £ is qualitatively the same, its difference being only quantitative. The characteristic feature is the same as for bulk crystals [24], £ has the form of a quasi-Lorentz function which is widening from the δ-peak at $T = 0$ K with increasing temperature and its maximum is weakly shifting into the region of lower energies.

At zero temperature $v_\lambda = 0$, thus $\Gamma_T = 0$ and $\Delta_T = \Delta_0 < 0$, i.e. as the energy zero the PE zone bottom ($E_0 = 0$) is taken, consequently the interaction with virtual phonons renormalizes the location of the PE zone bottom shifting it into the region of lower energies without any damping, i.e. the interaction with virtual phonons increases the PE binding energy not damping its basic state. From Fig. 2a, b it is clear that the exciton band is widening (Γ_T increases) and shifting into the region of smaller energies ($\Delta_T < 0$) as the temperature increases. Thus, the interaction with real phonons shifts the PE basic state into the long-wave spectrum region and the PE lifetime is decreasing.

Unlike the exciton function £ in bulk crystals in the PE function £ there is another characteristic maximum located in the high frequency region which is less intensive than the basic one. The described peculiarities of £(ξ) are caused by the specific interaction between the PE and the phonon modes of the heterosystem. The mechanism of interaction

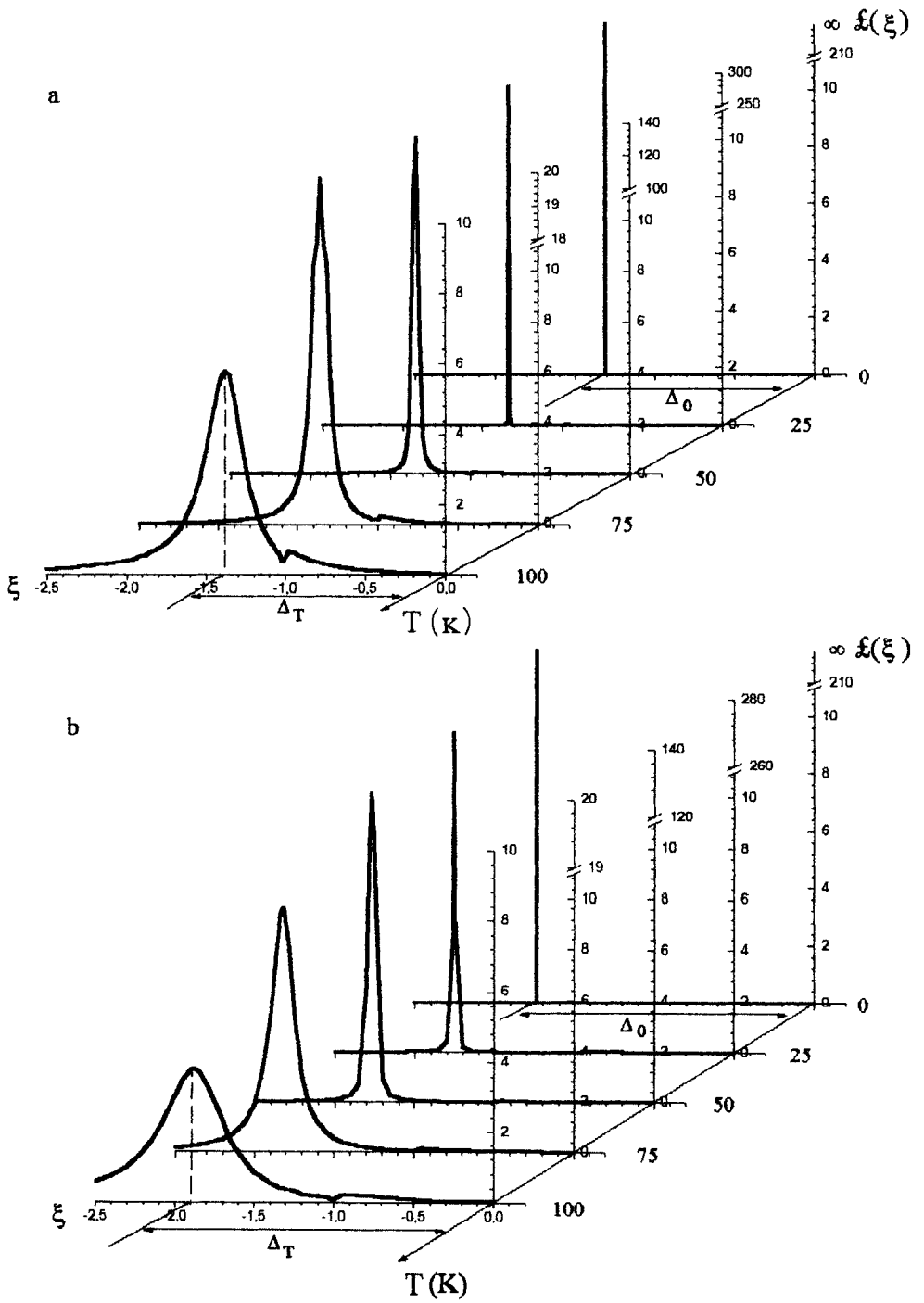

Fig. 2. Temperature dependence of the PE basic band shape function. a) $Cu_2O/TlBr$, b) $Cu_2O/SrTiO_3$ (ξ in units of Ω_{min})

is clear from the analysis of formulas (24) to (28) and Fig. 3, 4 which show the frequency dependence of all MO terms at $T = 0$ K and 100 K.

One can see that in the actual energy region (near the point ξ_0) at $T = 0$ K the interaction of the PE with the vibrations of all three modes takes place only in the processes of virtual

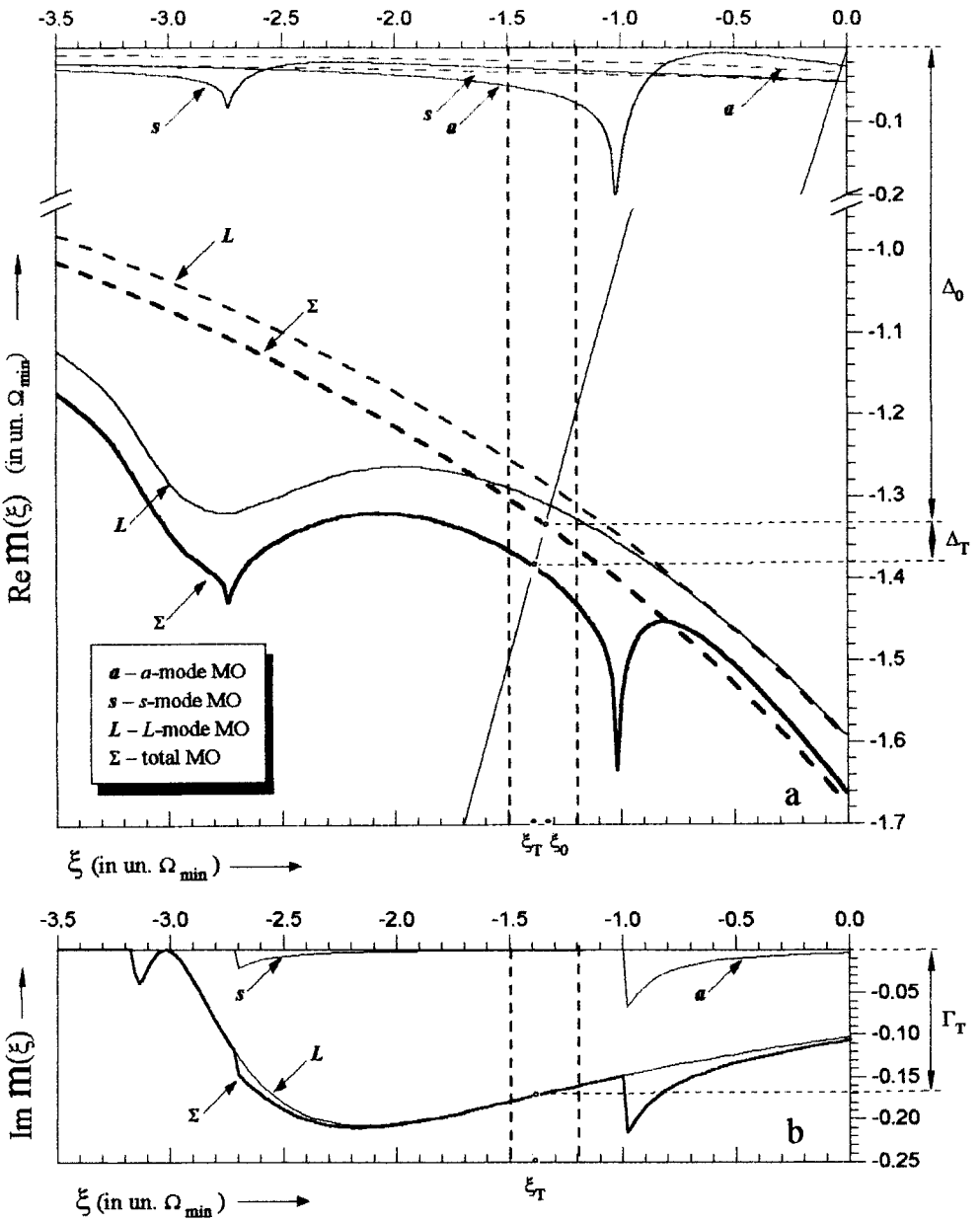

Fig. 3. Frequency dependence of the partial contributions a) Re $\mathfrak{m}_\lambda$, b) Im $\mathfrak{m}_\lambda$ and total values Re $\mathfrak{m}$ and Im $\mathfrak{m}$ in Cu_2O/TlBr. Dashed curves $T = 0$ K, solid curves $T = 100$ K

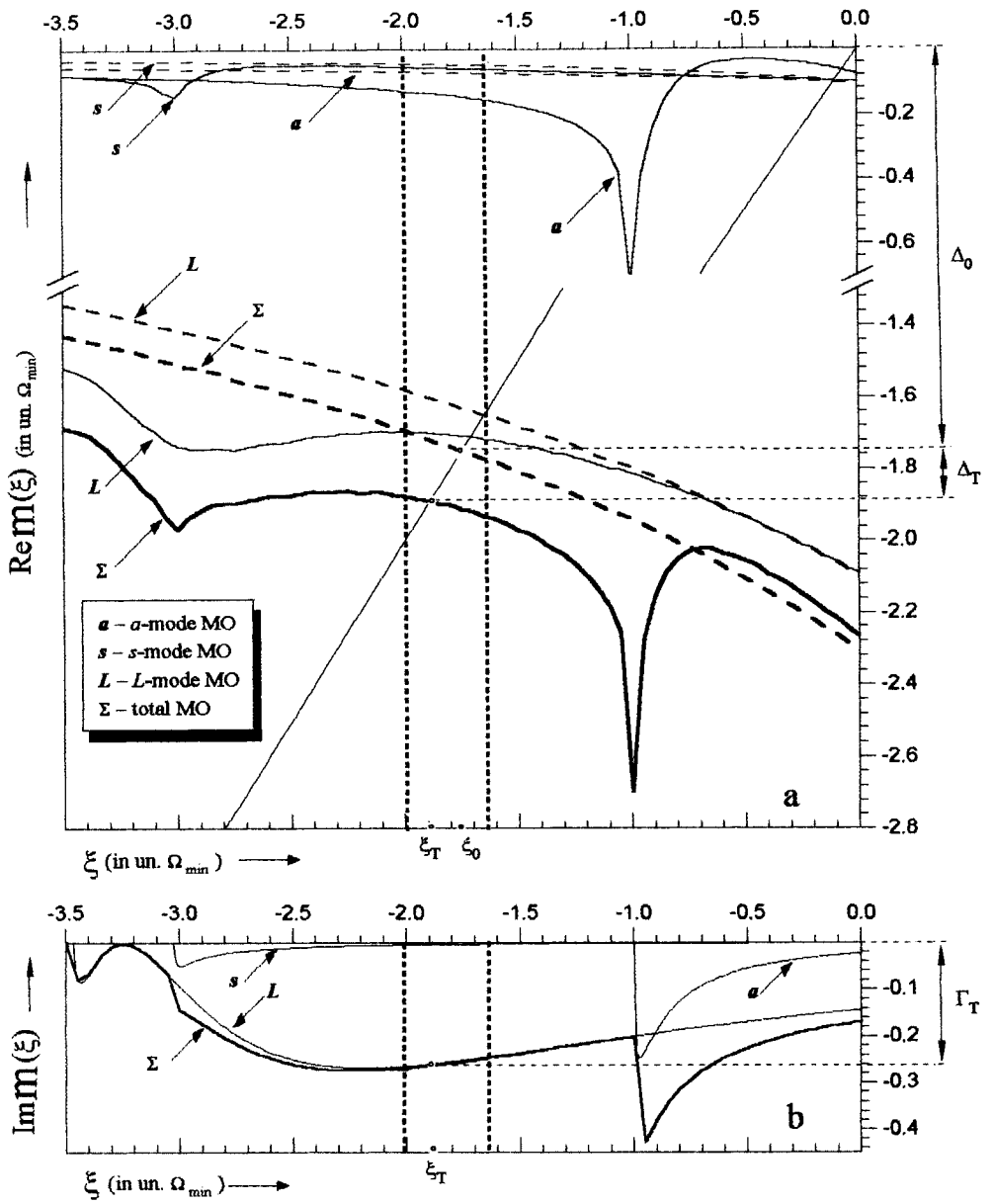

Fig. 4. Frequency dependence of the partial contributions a) Re $\mathbf{m}_\lambda$, b) Im $\mathbf{m}_\lambda$ and total values Re $\mathbf{m}$ and Im $\mathbf{m}$ in $Cu_2O/SrTiO_3$. Dashed curves $T = 0$ K, solid curves $T = 100$ K

phonon radiation (because in this case $\nu_\lambda = 0$). Due to the fact that these processes contribute to Re $\mathbf{m}(\xi)$ only when Im $\mathbf{m}(\xi \leqq 0) = 0$, it causes that £ has the δ-like form (Fig. 2a, b). Fig. 3, 4 show that the partial contributions of both presurface modes to the value of the total shift $\Delta_0 = \sum_\lambda \Delta_\lambda^0$ are smaller than that of the half-bulk mode.

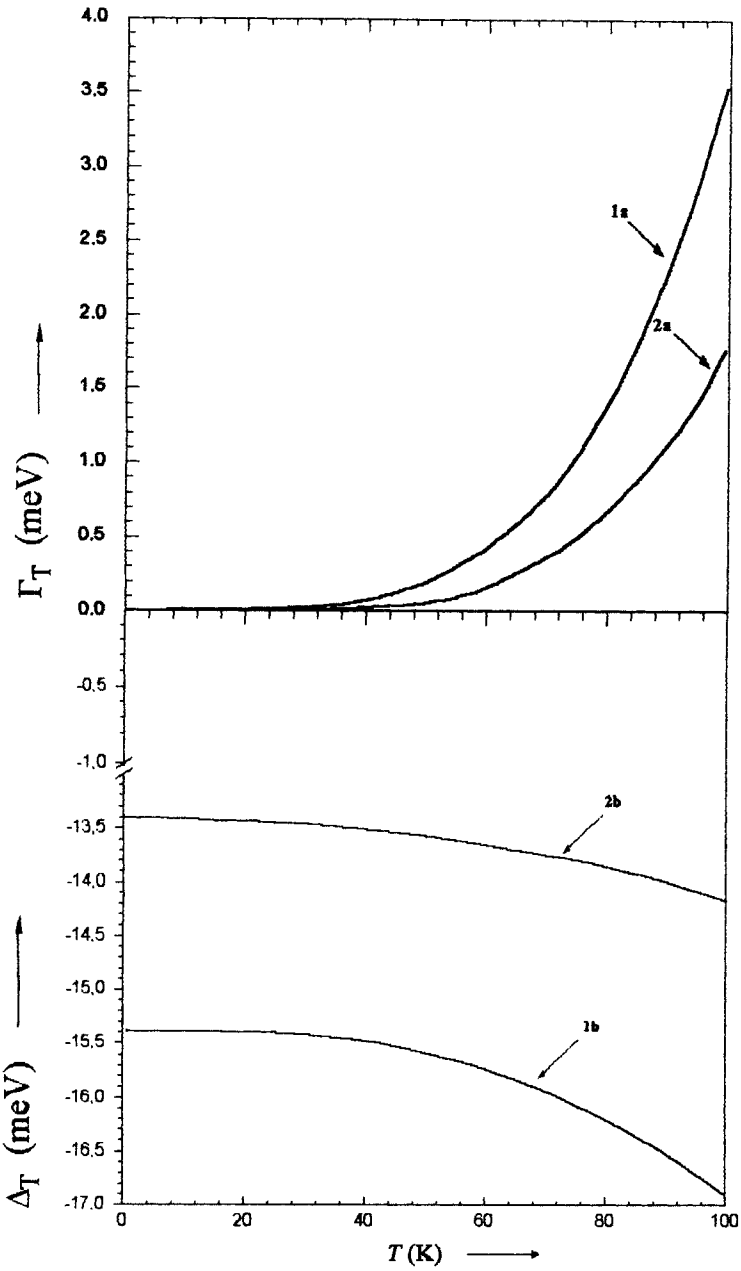

Fig. 5. Temperature dependence of shift (Δ_T) and half-width (Γ_T) of the PE basic band shape function. (1a, b) $Cu_2O/SrTiO_3$, (2a, b) $Cu_2O/TlBr$

So, as for the Wannier-Mott exciton [21] the zone bottom of the PE is renormalized mainly by longitudinally polarized phonons. The corresponding partial contributions of all modes to the total shift Δ_0 are bigger in the heterosystem where the dielectric constants $\varepsilon_0, \varepsilon_\infty$ are bigger ($Cu_2O/SrTiO_3$). This is clear because in this case the PE is

localized closer to the interface and therefore its interaction with all phonon modes increases.

At $T \neq 0$ K the average value of the phonon occupation numbers of all modes (ν_λ) differs from zero because the PE interacts not only with virtual phonons but also with real ones of all modes in the radiation processes as well as in the absorption processes. However, these processes influence the formation of £ parameters differently. Fig. 3, 4 show that in the actual region of energies (in Fig. 3, 4 it is confined by two vertical lines) all the three phonon modes make a contribution in $\mathrm{Re}\,\mathfrak{M}(\xi)$ to the both processes. So the temperature shift of the £ maximum according to the zone bottom renormalization (Δ_T) is due to all processes though the major contribution is made by the presurface a-phonons. Unlike the Wannier-Mott excitons where only LO-phonons cause the temperature shift Δ_T in the heterosystems these phonons give a smaller contribution to Δ_T though it is proportional to the presurface one. We can prove that despite the interaction between the PE and the presurface phonons is weaker than that with the bulk ones, but as $\Omega_a \approx \Omega_L/3$, at the fixed temperature $\nu_a \gg \nu_L$ and thus $\Delta_a^T > \Delta_L^T$.

Fig. 3, 4 show that in the actual energy region near the £ maximum the presurface phonons of the a-mode even in the absorption processes do not contribute to $\mathrm{Im}\,\mathfrak{M}(\xi)$ at all. However, s-mode phonons due to the weak interaction between them and the PE contribute much less than the half-bulk ones. Due to this fact the damping (half-width Γ) is defined by the interaction of the PE with the half-bulk phonons as it is true for Wannier-Mott excitons. The interaction processes between the PE and the absorption of real surface a-mode phonons lead to the considerable partial contributions in $\mathrm{Re}\,\mathfrak{M}(\xi)$ and $\mathrm{Im}\,\mathfrak{M}(\xi)$ in the region of energies higher than the energy of the renormalized zone bottom (ξ_T). This causes the appearance of an additional structure in the short-wave region of the £(ξ) function (see Fig. 2a, b). The spectral parameters for both heterosystems at nonzero temperatures have a qualitatively equal dependence as at $T = 0$ K. Only due to a stronger attraction of the PE to the interface in the heterosystem $Cu_2O/SrTiO_3$ all parameters have bigger magnitudes. The temperature dependence of the shift and half-width are given in Fig. 5.

We must point out once more that the obtained information on the shape function £ of the spectral zone of the PE is based on the one-phonon approximation for the MO and the neglect of the interzone interaction due to phonons. To make the obtained result more exact one has to take into consideration many-phonon processes and the PE zone structure to be perfect in future studies.

References

[1] T. ANDO, A. FOWLER, and F. STERN, Rev. mod. Phys. **54**, 437 (1982).
[2] C. CONSADORI and R. F. FRINDT, Phys. Rev. B **2**, 4893 (1970).
[3] C. KOLH, J. appl. Phys. **30**, 127 (1983).
[4] F. STERN and S. DAS SARMA, Phys. Rev. B **30**, 840 (1984).
[5] Y. KAYANUMA, Phys. Rev. B **38**, 9797 (1988).
[6] V. A. GOLOVATSKII and N. V. TKACH, Ukr. fiz. Zh. **33**, 1241 (1988).
[7] S. YU. KASANDROV, phys. stat. sol. (b) **162**, 435 (1990).
[8] R. S. KNOX, Theory of Excitons, Izd. Mir, Moscow 1966 (in Russian).
[9] L. WENDLER and B. HARTWIG, J. Phys. C **3**, 9907 (1991).
[10] L. WENDLER and E. JÄGER, phys. stat. sol. (b) **120**, 235 (1983).
[11] L. WENDLER, phys. stat. sol. (b) **129**, 513 (1985).
[12] L. WENDLER and R. PECHSTEDT, phys. stat. sol. (b) **141**, 129 (1987).

[13] L. WENDLER and R. HAUPT, phys. stat. sol. (b) **143**, 487 (1987).
[14] N. MORI and T. ANDO, Phys. Rev. B **40**, 6175 (1989).
[15] YU. E. LOZOVIK and V. N. NISHANOV, Fiz. tverd. Tela **18**, 3267 (1976).
[16] I. M. NEPOMNYASHI and V. N. NISHANOV, phys. stat. sol. (b) **126**, K53 (1984).
[17] V. V. PAZIUK and M. V. TKACH, phys. stat. sol. (b) **177**, 325 (1993).
[18] S. I. BERIL and E. P. POKATILOV, Fiz. Tekh. Poluprov. **14**, 37 (1980).
[19] S. I. BERIL, E. P. POKATILOV, and I. S. CHEBAN, Ukr. fiz. Zh. **27**, 585 (1982).
[20] A. S. DAVYDOV, Quantum Mechanics, 2nd ed., Pergamon Press, London/Oxford 1976.
[21] A. S. DAVYDOV, Solid-State Theory, Izd. Nauka, Moscow 1976 (in Russian).
[22] A. A. ABRIKOSOV, L. P. GORKOV, and I. E. DZYALOSHINSKI, Methods of Quantum Field Theory in Statistical Physics, Prentice Hall, Inc., Englewood Cliffs 1963.
[23] N. V. TKACH, Teor. mat. Fiz. **61**, 400 (1984).
[24] N. V. TKACH, Fiz. tverd. Tela **21**, 2506 (1979).