

INFLUENCE OF THE PARAMETER OF THE ELECTRON-PHONON INTERACTION ON THE ENERGY SPECTRUM OF POLARONS IN QUASI-TWO-DIMENSIONAL STRUCTURES

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We present the results of studies of the energy spectrum of polarons in quasi-two-dimensional heterosystems with a variable parameter of the electron-phonon interaction ($0 < \alpha < 3$) depending on the wave vector. The calculations were performed by using perturbation theory and the variational method of Lee-Low-Pines (LLP). The specific calculations were carried out for the heterostructures GaAs/AlAs, CdSe/glass, and CuCl/glass, for which the weak and intermediate electron-phonon couplings are realized: $\alpha = 0.071$, $\alpha = 0.0461$, and $\alpha = 2.091$, respectively. In the frames of the LLP method, the wave function of a polaron is determined. We evaluated the mean number of virtual phonons surrounding an electron, calculated the binding energy of a polaron and its effective mass as a function of the wave vector, and performed the comparative analysis of structures with different electron-phonon couplings.

The investigation of semiconductor nanoheterostructures is one of the perspective directions of the development of solid state physics. This is related not only to the interesting physical properties of spatially bounded structures, but to their important applied potentialities in the design of novel lasers and computers of the new generation.

The physical properties of superthin films of semiconductors which are in contact with two media, double heterostructures of semiconductors, differ from those of the corresponding single crystals by changes of the energy spectra of charged particles (electrons, holes) and the oscillation spectra of atoms.

The investigations of the electron-phonon interaction are carried out in a great number of experimental and especially theoretical works [1–3]. To a great extent, this concerns also the physics of nanoheterosystems [4–13].

The most known are two methods of theoretical studies: perturbation theory [2, 3] and the LLP method which is grounded on certain unitary transformations. The theory of polaron states is quite well developed for massive three-dimensional crystals characterized by the translational symmetry. In particular, it is known that

these methods allow one to get quite good results for the polaron states with small wave vectors. Moreover, the perturbation theory gives the proper value of the binding energy of a polaron state and the effective mass for small values of the constant of the electron-phonon interaction ($\alpha \ll 1$), whereas the LLP method can be used for $\alpha \leq 6$ [3]. As for the dispersion law of a polaron for $k > 0$, the mentioned methods can be applied with certain precautions [2], especially for the values of k , at which the electron energy is close to the phonon energy ($k = k_f = (\frac{2m\omega}{\hbar})^{1/2}$). More universal in this aspect is the method of Green functions [4, 6, 14] which allows one, with regard for the main diagrams, to calculate the polaron energy with high accuracy for the whole spectrum. But, in so doing, one frequently meets quite complicated mathematical difficulties [2].

In studying the nanoheterosystems, for which the translational symmetry is broken for three, two, or one direction, the theory of polaron states becomes more complicated. This is related to changes in the phonon and electron energy spectra [4] and in the electron-phonon interaction [8] in heterosystems. Thus, the problems concerning the dependence of the dispersion law for polarons on the main parameters of the system remain to be insufficiently studied. It is also important to investigate the influence of a choice of the method of solution of the polaron problem on the derived results.

This work is devoted to the study of the polaron energy as a function of the wave vector for quasi-two-dimensional heterosystems with different values of the electron-phonon interaction ($0 < \alpha < 3$). To this end, we use perturbation theory and the variational LLP method. For heterosystems of the type GaAs/AlAs, CdSe/glass, and CuCl/glass with a quantum well, we also calculated the binding energy of a polaron and its effective mass as a function of the wave vector.

1. Statement of the Problem. General Formulas

We consider a heterostructure with two plane boundaries, in which longitudinal optical phonons interact with a conduction band electron. The Hamiltonian of such a system is as follows:

$$\hat{H} = \hat{H}_e + \hat{H}_{\text{ph}} + \hat{H}_{\text{int}}. \quad (1)$$

The energy operator of an electron located in the potential well can be represented as

$$\hat{H}_e = \frac{\hat{p}_{\parallel}^2}{2m_{\parallel}} + \frac{\hat{p}_{\perp}^2}{2m_{\perp}} + V(z), \quad (2)$$

where \hat{p}_{\parallel} and \hat{p}_{\perp} are, respectively, the operators of momentum of an electron in the xy plane and in the direction along the z axis of the Cartesian coordinate system, m_{\parallel} and m_{\perp} are the corresponding effective masses of an electron, and $V(z)$ is the potential energy of an electron located in the rectangular potential well

$$V(z) = \begin{cases} 0, & 0 < z < L \\ V_0, & z \leq 0, z \geq L \end{cases}. \quad (3)$$

The operators describing the system of phonons \hat{H}_{ph} and the electron-phonon interaction can be written in the occupation number representation in terms of the phonon-related variables as

$$\hat{H}_{\text{ph}} = \sum_{\vec{q}} \hbar\omega \left(b_{\vec{q}}^{\dagger} b_{\vec{q}} + \frac{1}{2} \right), \quad (4)$$

$$\hat{H}_{\text{int}} = \sum_{\vec{q}} \left\{ V_{\vec{q}} b_{\vec{q}} + V_{\vec{q}}^* b_{\vec{q}}^{\dagger} \right\}, \quad (5)$$

where is the operator of annihilation of a phonon with energy $\hbar\omega$ and wave vector \vec{q} . For the heterosystem, the function of the electron-phonon interaction $V_{\vec{q}}$ looks as

$$V_{\vec{q}} = -\frac{\hbar\omega i}{q} \left(\frac{\hbar}{2m_e\omega} \right)^{1/4} \left(\frac{4\pi\alpha}{SL} \right)^{1/2} e^{i\vec{q}_{\parallel}\vec{r}_{\parallel}} \sin\left(\frac{\pi}{L}nz\right), \quad (6)$$

where

$$m_e = \sqrt{m_{\parallel}m_{\perp}}, \quad \alpha = \frac{e^2}{2\hbar c} \left(\frac{2m_e c^2}{\hbar\omega} \right)^{1/2} \left(\frac{1}{n^2} - \frac{1}{\varepsilon} \right)$$

is the constant of the electron-phonon interaction [1], and S is the interface area of the media.

The chosen Hamiltonian of the electron-phonon subsystem does not take into account the presence of interface polarization phonons. Such an approximation is valid only for a quantum well, whose size is greater than the radius of a polaron.

Taking into account the fact that the heterosystem under study is an intermediate system between a three-dimensional (3D) massive crystal and a two-dimensional (2D) system, we will compare the derived results for the heterosystem with the relevant ones for 3D- and 2D-systems. The function $V_{\vec{q}}$ for a 3D-system is well known:

$$V_{\vec{q}} = -\frac{\sqrt{4\pi\alpha}(\hbar\omega i)}{\sqrt{LSq^2}} \left(\frac{\hbar}{2m_e\omega} \right)^{1/4} e^{i\vec{q}\vec{r}}; \quad (7)$$

for a 2D-system, it reads

$$V_{\vec{q}} = -\frac{\sqrt{2\pi\alpha}(\hbar\omega i)}{\sqrt{Sq_{\parallel}}} \left(\frac{\hbar}{2m_e\omega} \right)^{1/4} e^{i\vec{q}_{\parallel}\vec{r}_{\parallel}}. \quad (8)$$

To evaluate the polaron energy, we used both perturbation theory and the LLP method. By using the latter, we took into account that the system under consideration includes fast and slow subsystems. As the former, we consider the movement of an electron in the direction normal to the interface. Therefore, we use the adiabatic approximation: the given Hamiltonian is averaged on the wave functions of the ground stationary state for the movement along the OZ axis:

$$\hat{H}_{\text{eff}} = \langle \psi_1(z) | \hat{H} | \psi_1(z) \rangle, \quad (9)$$

Here, the function $\psi_n(z)$ is a solution of the Schrödinger equation

$$\left[-\frac{\hbar^2}{2} \frac{d}{dz} \frac{1}{m_{\perp}} \frac{d}{dz} + V(z) \right] \psi_n(z) = E_n \psi_n(z), \quad (10)$$

$n = 1, 2, 3, \dots$

To Hamiltonian (9), we applied successively two unitary transformations by using the operators

$$\hat{S} = \exp \left[\frac{i}{\hbar} \left(\vec{P} - \sum_{\vec{q}_{\parallel}} b_{\vec{q}}^{\dagger} b_{\vec{q}} \hbar \vec{q}_{\parallel} \right) \vec{r}_{\parallel} \right], \quad (11)$$

$$\hat{U} = \exp \left\{ \sum_{\vec{q}} \left(b_{\vec{q}}^{\dagger} f(\vec{q}) - b_{\vec{q}} f^*(\vec{q}) \right) \right\}. \quad (11a)$$

In view of the well-known relations for the unitary transformations of the operators $b_{\vec{q}}$ and $b_{\vec{q}}^\dagger$, we averaged over the vacuum phonon state $|0\rangle$ and got the energy function for the electron-phonon system as

$$\begin{aligned} \varepsilon(f) &= \langle 0|U^{-1}HU|0\rangle = \\ &= E_1 + \frac{P^2}{2m_e} + \sum_{\vec{q}} \{V_{\vec{q}}M_{11}f(\vec{q}) + V_{\vec{q}}^*M_{11}^*f(\vec{q})\} + \\ &+ \frac{\hbar^2}{2m_e} \left\{ \sum_{\vec{q}} |f(\vec{q})|^2 \vec{q} \right\}^2 + \\ &+ \sum_{\vec{q}} |f(\vec{q})|^2 \left\{ \hbar\omega - \frac{\vec{q}\vec{P}}{m_e}\hbar + \frac{q^2}{2m_e}\hbar^2 \right\}, \end{aligned}$$

where $M_{1n} = \int_{-\infty}^{\infty} \psi_1(z) e^{iqz} \psi_n(z) dz$, $n = 1, 2, \dots$

By minimizing $\varepsilon(f)$ in $f(\vec{q})$ and $f^*(\vec{q})$ and by considering that $\vec{P} = \hbar\vec{k}$, we got the polaron energy in the heterosystem. It is convenient to reckon the polaron energy from the size-quantization level E_1 :

$$\begin{aligned} E_{\text{pol}}(k) &= \frac{\hbar^2 k^2}{2m_e} (1 + \eta^2) + \sum_{\vec{q}} \frac{-2|V_{\vec{q}}|^2 |M_{11}|^2}{\hbar\omega - \frac{\hbar\vec{q}\vec{P}}{m_e} (1 - \eta) + \frac{\hbar^2 q^2}{2m_e}} + \\ &+ \sum_{\vec{q}} \frac{|V_{\vec{q}}|^2 |M_{11}|^2 \left\{ \hbar\omega - \frac{\hbar\vec{q}\vec{P}}{m_e} + \frac{\hbar^2 q^2}{2m_e} \right\}}{\left\{ \hbar\omega - \frac{\hbar\vec{q}\vec{P}}{m_e} (1 - \eta) + \frac{\hbar^2 q^2}{2m_e} \right\}^2}, \end{aligned} \quad (12)$$

where

$$\eta\vec{P} = \sum_{\vec{q}} |f_{\min}(\vec{q})|^2 \hbar\vec{q}_{\parallel},$$

$$f_{\min}(\vec{q}) = - \frac{V_{\vec{q}}^* M_{11}^*}{\hbar\omega + \frac{\hbar^2 q_{\parallel}^2}{2m_e} - \frac{\hbar^2}{m_e} \vec{k}\vec{q}_{\parallel} (1 - \eta)}.$$

Relation (12) differs from the corresponding formulas for 3D- and 2D-systems by the presence of the function $M_{1n}(\vec{q}_z)$ which appears due to the breaking of the translational symmetry in the heterosystem.

For the weak electron-phonon coupling, the polaron energy can be determined with the use of perturbation theory as

$$E_{\text{pol}}^{(\vec{k})} = \frac{\hbar^2 k^2}{2m_e} + \sum_{\vec{q}_{\parallel}, n} \frac{|V_{\vec{q}}|^2 |M_{1n}|^2}{E_1 - E_n - \hbar\omega - \frac{\hbar^2 q_{\parallel}^2}{2m_e} + \frac{\hbar^2 \vec{q}_{\parallel} \vec{k}}{m_e}}. \quad (13)$$

As distinct from the LLP method, the adiabatic approximation was not applied upon the derivation of (13). In this approximation, formula (13) is simplified:

$$E_{\text{pol}}^{(\vec{k})} = \frac{\hbar^2 k^2}{2m_e} + \sum_{\vec{q}_{\parallel}} \frac{|V_{\vec{q}}|^2 |M_{11}|^2}{-\hbar\omega - \frac{\hbar^2 q_{\parallel}^2}{2m_e} + \frac{\hbar^2 \vec{q}_{\parallel} \vec{k}}{m_e}}. \quad (13')$$

Expressions (12) and (13) describe the dependence of the polaron energy on the wave vector, i.e. the dispersion law for a polaron.

2. Numerical Calculations. Analysis of the Results

In the majority of works (see, e.g., [1, 2, 7]), the region of small values of the wave vector ($k \approx 0$) is usually considered. Therefore, the quantities $\eta(k)$ and $E_{\text{pol}}(k)$ are determined upon the expansion of the relevant expressions in series, by taking only their first terms. Here, we consider the region of wave vectors where the electron does not create a real phonon:

$$0 \leq k < k_f, \quad k_f = \sqrt{\frac{2m_e\omega}{\hbar}}.$$

This value of the wave vector is significantly lesser than its boundary value in the Brillouin zone: $k_f \ll \ll k_0 = \frac{\pi}{a}$.

The specific calculations were carried out for the heterostructure GaAs/AlAs and model heterostructures CdSe/glass and CuCl/glass, for which the weak and intermediate electron-phonon couplings are realized: $\alpha = 0.071$, $\alpha = 0.0461$, and $\alpha = 2.091$, respectively. Two last heterostructures were first experimentally derived and investigated in the case of quasi-zero-dimensional systems [16–18].

Upon the study of the problem concerning polarons in nanoheterosystems, the adiabatic approximation is frequently in use [10, 11]. With the purpose to determine the region of thicknesses L , for which the adiabatic approximation can be used, we calculated the polaron energy at $k = 0$ for various values of L for the heterosystem GaAs/AlAs according to formulas (13) and (13'). The results of calculations are given in Fig. 1. It is seen for the given heterosystem that the error is at most 13% for $L < 100 \text{ \AA}$ and is 2% at $L = 20 \text{ \AA}$. Therefore, the calculations were performed for $20 \text{ \AA} \leq L \leq 100 \text{ \AA}$.

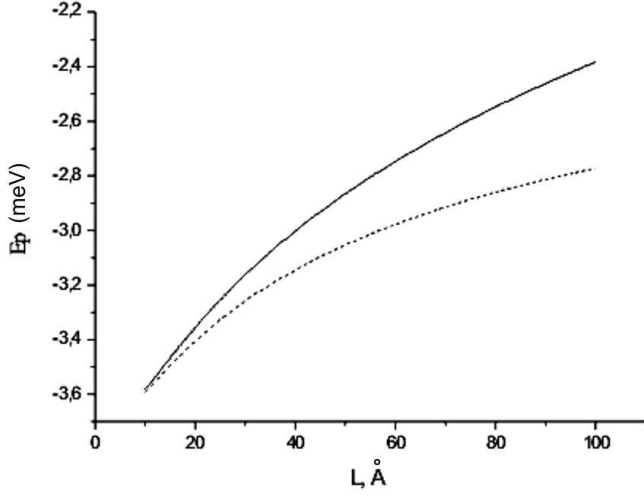


Fig. 1. Energy $E_p(0)$ versus L for the heterosystem GaAs/AlAs according to perturbation theory (the dotted line – the adiabatic approximation)

In the frames of the LLP method, we define the wave function of a polaron as

$$\psi_{\text{pol}}(r) = \exp \left\{ i \left(\vec{k} - \sum_{\vec{q}} b_{\vec{q}}^{\dagger} b_{\vec{q}} \right) \cdot \vec{r} \right\} \times \exp \left\{ \sum_{\vec{q}} b_{\vec{q}}^{\dagger} f_{\text{min}}(\vec{q}) - b_{\vec{q}} f_{\text{min}}^*(\vec{q}) \right\} |0\rangle. \quad (14)$$

As seen from formula (12), function (14) is defined by an auxiliary function η which depends on the wave vector \vec{k} . The executed calculations of the function $\eta = \eta(k)$ for a massive crystal, 2D-system, and heterosystems with different crystals and different widths of a quantum well showed that it is constant only in the region of very small k [1] and monotonously grows with k . Moreover, for a given k , the values of the function $\eta = \eta(k)$ increase with decrease in the width of a quantum well. This dependence is presented in Fig. 2 for a CuCl crystal.

If the function $\eta = \eta(k)$ is known, we can define the mean number of virtual phonons surrounding an electron as

$$n = n(k) = \langle \psi^* | \sum_{\vec{q}} b_{\vec{q}}^{\dagger} b_{\vec{q}} | \psi \rangle = \sum_{\vec{q}} |f_{\text{min}}(\vec{q})|^2. \quad (15)$$

In Fig. 3, we present the functions $n = n(k)$ for a massive 2D crystal CuCl and the heterosystem CuCl/glass.

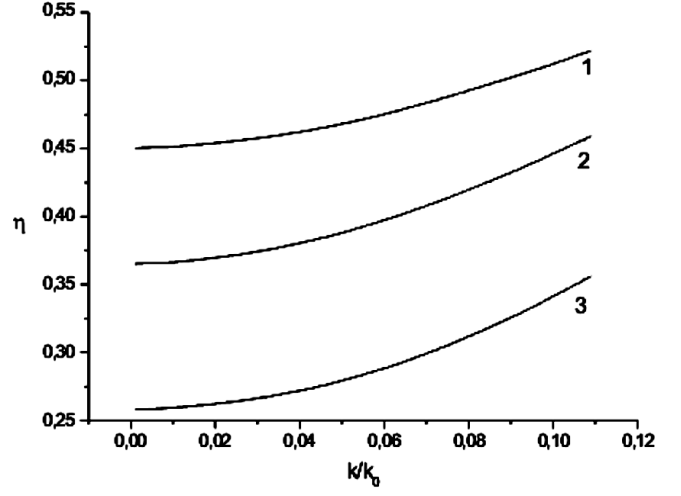


Fig. 2. Functions $\eta = \eta(k)$: 1 – 2D-structure, 3 – 3D-structure, 2 – heterostructure CuCl/glass with $L = 25 \text{ \AA}$

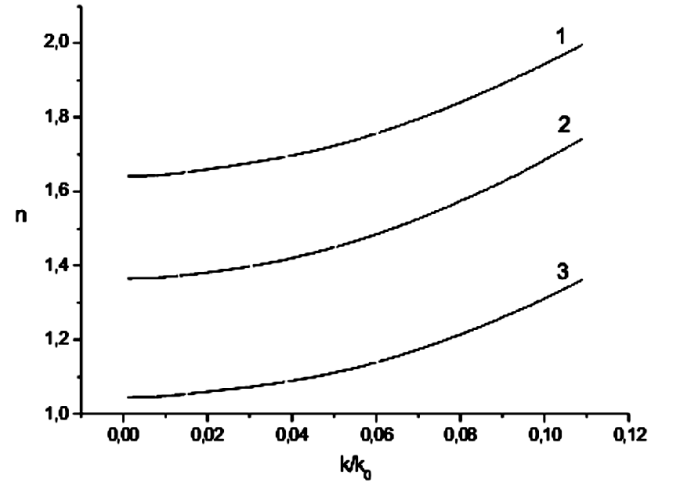


Fig. 3. Mean number of virtual phonons: 1 – 2D-structure, 3 – 3D-structure, 2 – heterostructure CuCl/glass with $L = 25 \text{ \AA}$

The function $n = n(k)$ increases monotonously with k . Moreover, we observe the parabolic behavior in the region of small k . The increase in k is accompanied by a deviation of the function $n = n(k)$ from the parabolic behavior.

In order to determine the dispersion law of a polaron, $E_{\text{pol}} = E_{\text{pol}}(k)$, it is necessary to pass from the summation to the integration in the relevant formulas (12) and (13) and to perform the specific calculations with the use of a computer. For a 3D-system in the

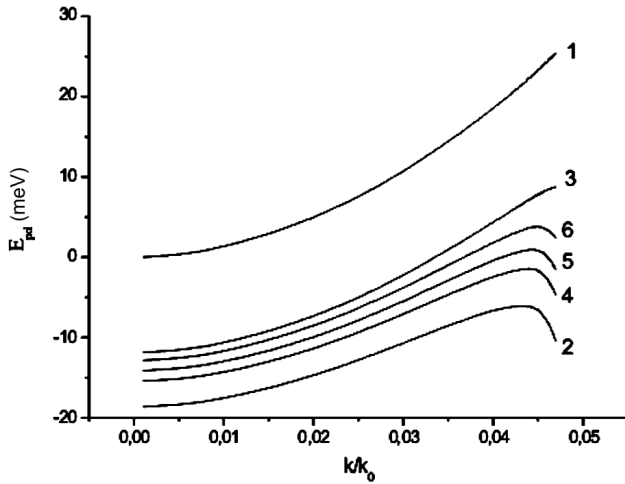


Fig. 4. Polaron energies for a crystal CdSe and the heterostructure CdSe/glass. 1 – the electron energy, 2, 3 – 2D- and 3D-systems of a crystal CdSe, 4, 5, 6 – heterosystems CdSe/glass with quantum wells with widths of 25, 50, and 100 Å, respectively

frames of perturbation theory, the dispersion law can be derived in the analytic form:

$$E_{\text{pol}}^{3D}(k) = -\alpha \frac{\hbar^2}{2m_e} k_f^2 \frac{\arcsin \frac{k}{k_f}}{\frac{k}{k_f}}. \quad (16)$$

In the region of small wave vectors, formula (16) yields the well-known result

$$E_{\text{pol}}^{3D}(0) = -\alpha \hbar \omega \quad (17)$$

which coincides with that derived by the LLP method. For a 2D-system, formula (8) allows us to deduce the dispersion law for polarons. It can be also written in the analytic form as

$$E_{\text{pol}}^{2D}(k) = -\frac{\alpha}{4} \hbar \omega_0 F\left(2\pi, \frac{k}{k_f}\right), \quad (18)$$

where $F\left(2\pi, \frac{k}{k_f}\right)$ is the elliptic integral of the first kind [18].

Let $k \approx 0$. After simple transformations, the polaron energy is reduced to the form

$$E_{\text{pol}}^{2D}(0) = -\frac{\pi\alpha}{2} \hbar \omega_0. \quad (19)$$

In Fig. 4, we give the function $E_p = E_p(k)$ for a crystal CdSe. Besides the polaron energy (curves 2–6), we present the dependence for a “bare” electron (curve 1).

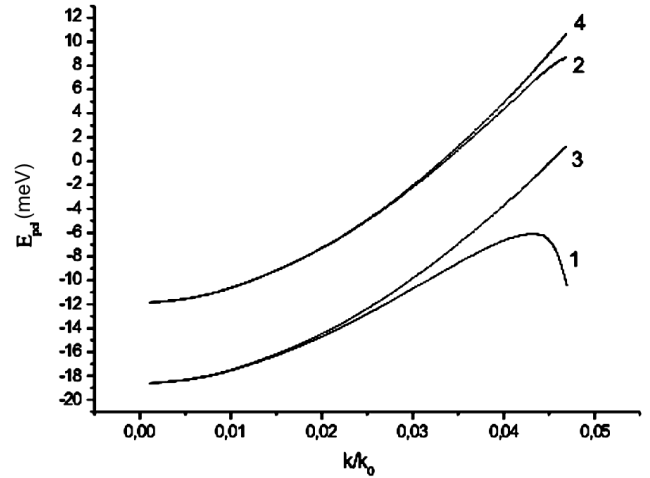


Fig. 5. Polaron energy (for the heterostructure CdSe/glass); curves 1, 2 – the polaron energy of 2D- and 3D-structures, respectively, calculated according to perturbation theory, curves 3, 4 – the polaron energy in 2D- and 3D-structures, respectively, calculated by the LLP method

The given plots indicate that the dispersion law has parabolic character in the region of small wave vectors for a massive crystal and for a quasi-two-dimensional system (a heterosystem) or a 2D-crystal. The increase in the wave vector changes the dependence $E_p = E_p(k)$. Each dispersion curve is characterized by the point of inflection (k_p) and by the point of maximum (k_m). A decrease in the dimensionality of the system leads to a decrease in numerical values of k_p and k_m .

The analogous calculations for $E_p = E_p(k)$ were performed by the LLP method. For small wave vectors ($k \approx 0$), we get practically the same dependence as by perturbation theory. The increase in the value of the wave vector is accompanied by the growth of the deviation between the results of both methods. In Fig. 5, we give only the dispersive curves for 3D- 2D-systems for the sake of clearness. In the region under consideration ($k \leq k_f$) for a fixed k , the decrease in the dimensionality of a crystalline system increases the difference between the values of the polaron energy derived with the use of perturbation theory and the LLP method.

The calculation performed for the heterosystem CuCl/glass and a crystal CuCl, which is characterized by a greater electron-phonon interaction, indicates that the dispersion laws are qualitatively analogous to that for a crystal CdSe. But the difference between the results of two methods of calculations for the CuCl-heterosystems is greater than that for the CdSe-based ones.

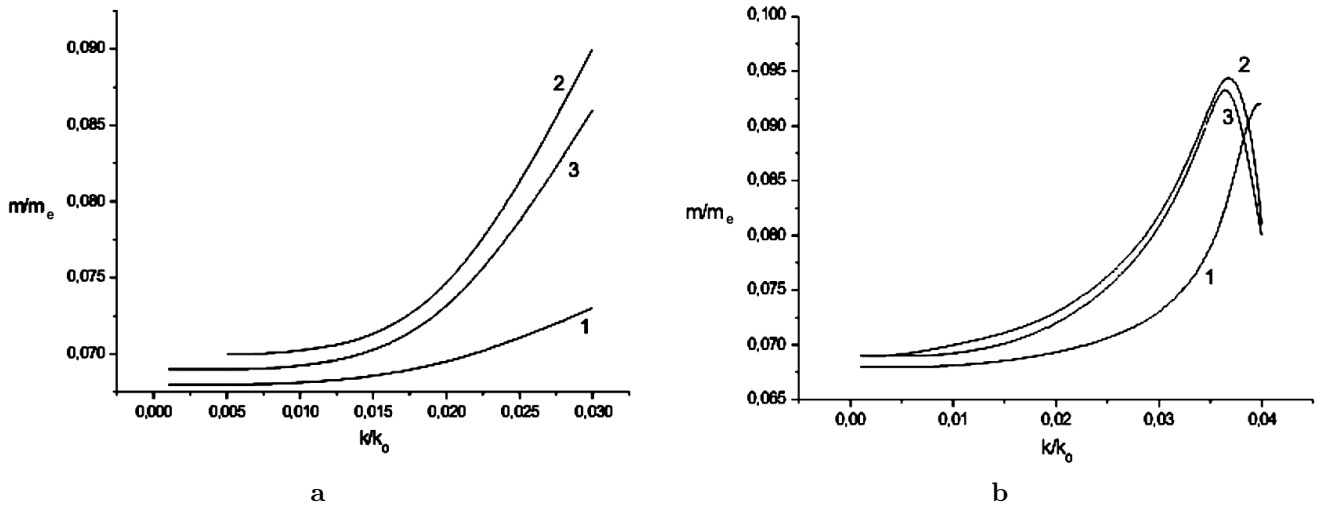


Fig. 6. Dependences $m_p = m_p(k)$ according to perturbation theory (curves a) and the LLP method (curves b): 1 – 3D-crystal GaAs; 2 – 2D-crystal GaAs; 3 – heterosystem GaAs/AlAs with $L = 25 \text{ \AA}$

More obvious is the difference between the results of calculations according to perturbation theory and the LLP method for the parameter called by the effective polaron mass which is defined by the second derivative of the function $E_{\text{pol}} = E_{\text{pol}}(k)$:

$$m_p^{-1} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k^2}.$$

In Fig. 6, we present the dependences $m_p = m_p(k)$ for the heterosystem GaAs/AlAs. In the region of small k , both methods give the same results. But the increase in k leads to the growth of the difference of the functions $m_p = m_p(k)$ derived by different methods. In particular, $m_p = m_p(k)$ tends to infinity according to perturbation theory (Fig. 6,a) as $k \rightarrow k_p$, which is understandable, since k_p is the point of inflection in the relevant plots $E_{\text{pol}} = E_{\text{pol}}(k)$ (Fig. 4). The function $m_p = m_p(k)$ derived by the LLP method is smoother and reaches the maximum value in the region $k \approx k_p$.

Thus, we have studied the energy spectrum of a polaron in certain quasi-two-dimensional heterosystems with the variable parameter of the electron-phonon interaction ($0 < \alpha < 3$) depending on the wave vector. The calculations were performed by using perturbation theory and the variational method of Lee–Low–Pines. The specific calculations were carried out for the heterostructures GaAs/AlAs, CdSe/glass, and CuCl/glass, for which the weak and intermediate electron-phonon couplings are realized: $\alpha = 0.071$, $\alpha =$

0.0461 , and $\alpha = 2.091$, respectively. In the frames of the LLP method, we have determined the wave function of a polaron, calculated the mean number of virtual phonons surrounding an electron, evaluated the binding energy of a polaron and its effective mass as a function of the wave vector, and carried out the comparative analysis of the structures with different electron-phonon couplings.

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ВПЛИВ ПАРАМЕТРА ЕЛЕКТРОН-ФОНОННОЇ ВЗАЄМОДІЇ НА ЕНЕРГЕТИЧНИЙ СПЕКТР ПОЛЯРОНІВ КВАЗІДВОВИМІРНИХ СТРУКТУР

В.І. Бойчук, В.А. Борусевич

Резюме

Наведено результати дослідження енергетичного спектра полярона квазідвовимірних гетеросистем з різною величиною параметра електрон-фононої взаємодії ($0 < \alpha < 3$) в залежності від хвильового вектора. Обчислення проведено за допомогою двох методів: теорії збурень та варіаційного методу Лі—Лоу—Пайнса (ЛЛП). Конкретні обчислення проведено для гетероструктур GaAs/AlAs, CdSe/скло і CuCl/скло, для яких реалізується слабкий і проміжний електрон-фононний зв'язок: $\alpha = 0,071$, $\alpha = 0,0461$ і $\alpha = 2,091$ відповідно. У рамках методу ЛЛП визначено хвильову функцію полярона. Визначено також середнє число віртуальних фононів, що охоплюють електрон. Обчислено енергію зв'язку полярона та його ефективну масу як функції хвильового вектора. Зроблено порівняльний аналіз структур з різним електрон-фононним зв'язком.