PHONON AND POLARON STATES OF A QUANTUM WELL HETEROSTRUCTURE OF CRYSTALS WITH A HEXAGONAL LATTICE STRUCTURE

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Abstract

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Keywords: nanoheterostructure, quantum well, electron-phonon interaction, polaron, perturbation theory, variational method

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Introduction

In the last two decades main results in physics of semiconductor heterostructures are related to a considerable degree to investigations of the electron-optical phonon interaction. The electron-phonon interaction is decisive in the analysis of electron scattering, energy exchange between hot electrons and the lattice, polaron effects etc. In most reports this interaction is based on the dielectric continuum model (DCM). The use of DCM makes it possible to obtain relatively simple analytical expressions for different physical quantities [1]. In addition, the results received within the framework of the DC model are in good agreement with the data of detail microscopic calculations [2,3] and experiment [4,5].

The electron-phonon interaction is investigated sufficiently well in different low-dimensional systems: quasi-two-dimensional heterostructures, quantum wires and quantum dots made from optically isotropic materials. However, in recent years anisotropic materials such as ZnO, GaN, AlN, and InN draw physicists’ attention because of their application in electronics. Therefore, in the dielectric continuum model optical phonons and their interaction with an electron in heterostructures with one [7] and two interfaces [7-9], infinite superlattices [10], and also different multilayer heterostructures [11,12] are examined. Theoretical researches stimulated a number of experimental works which involved the measurement of the Raman spectra of heterosystems [13-16].

As a rule, theoretical studies consider symmetric heterosystems where a nanofilm of one crystal is
adjacent to identical media (e.g., AlN/GaN/AlN). Such a structure is a partial case of the asymmetric three-layer heterosystem in which semi-confined media are different.

The purpose of the work is a theoretical analysis of the polarization phonon and polaron dispersion relations in the double nanoheterostructure of hexagonal lattice structure crystals.

1. Statement of the problem. General formulas

A three-layer planar heterostructure with a nanofilm of thickness \( L \) between two semi-infinite media is considered (Fig. 1). The coordinate system is chosen in such a way that the crystallographic axis \( C \) coincides with the \( z \)-axis. The separation boundaries of the heterosystem are given by

\[
|z| = \frac{L}{2}.
\]

| material 1 | material 2 | material 3 |
|------------|------------|------------|
| \( \varepsilon_1(\omega) \) | \( \varepsilon_2(\omega) \) | \( \varepsilon_3(\omega) \) |

If continuity of the potential and normal component of the induction vector is taken into account, one can obtain the conditions

\[
\Phi \left( \frac{L}{2} \right) = \Phi \left( -\frac{L}{2} \right),
\]

\[
\Phi \left( \frac{L}{2} \right) = \Phi \left( -\frac{L}{2} \right).
\]

\[
\varepsilon_{zz} \frac{\partial \Phi}{\partial z} \bigg|_{z=\pm L/2} = \varepsilon_{zz} \frac{\partial \Phi}{\partial z} \bigg|_{z=\pm L/2},
\]

\[
\varepsilon_{zz} \frac{\partial \Phi}{\partial z} \bigg|_{z=\pm L/2} = \varepsilon_{zz} \frac{\partial \Phi}{\partial z} \bigg|_{z=\pm L/2}.
\]

In the wurtzite-based crystals there exist two phonon types: ordinary and extraordinary. The first phonon type is quanta of transverse oscillations non-interacting with an electron. Extraordinary phonons are characterized by the fact that \( \tilde{E} \) is parallel to \( \tilde{Q} \) and they interact with electrons, e.g., by creating polaron states. Therefore, we further consider only the properties of extraordinary phonons.

From Eq. (1) it is easy to get the dispersion relation of extraordinary phonons in a bulk crystal,

\[
e_{\perp}(\omega)Q^2 + e_{\parallel}(\omega)q^2 = 0.
\]

The phonon energy spectrum in the heterostructure is based on the analysis of Eq. (3). It is seen that a general solution of the equation is expressed

\[
\Phi(z) = A e^{\chi z} + B e^{-\chi z}, \quad \chi = \sqrt{\frac{\varepsilon_{zz}(\omega)}{\varepsilon_{zz}(\omega)}} q.
\]

If \( \varepsilon \varepsilon_{\perp} < 0 \), one obtains solutions for oscillating phonon waves. And if \( \varepsilon \varepsilon_{\parallel} > 0 \), phonon waves are decaying (\( \chi \) is a real quantity).

For the heterostructures of crystals with a hexagonal lattice structure there can exist confined, interface half-space, and propagating phonons.

Confined polarization phonons are characterized with oscillating solutions for \( \Phi(z) \) inside \((-\frac{L}{2} \leq z \leq \frac{L}{2})\) and decaying solutions outside the nanofilm: \(|z| > \frac{L}{2}\). Thus, in order for confined polarization vibrations to exist, the following conditions must be satisfied:

\[
e_{zz} \varepsilon_{zz} < 0, \varepsilon_{\parallel} \varepsilon_{\parallel} > 0, \varepsilon_{\parallel} \varepsilon_{\parallel} > 0.
\]
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\[ \Phi(z) = \begin{cases} \Phi_1(z), & z < -L/2 \\ \Phi_2(z), & |z| \leq L/2 \\ \Phi_3(z), & z > L/2 \end{cases} \]

the quantities \( \Phi_1(z), \Phi_2(z), \Phi_3(z) \) are written

\[ \Phi_1(z) = A_1 e^{\chi(z)} \cos(kz) + B_1 e^{\chi(z)} \sin(kz), \]

\[ \Phi_2(z) = A_2 \cos(kz) + B_2 \sin(kz), \]

\[ \kappa_z = \frac{e_{1z}}{e_{2z}}, \]

\[ \Phi_3(z) = B_3 e^{\chi(z)} \cos(kz), \]

By substituting (9)–(11) in Eq. (4), one can obtain the system of homogeneous equations over coefficients \( A_1, A_2, B_2, B_3 \). Since these coefficients are different from zero, we receive the equation for the wave vector \( q \) and frequency \( \omega \):

\[ \begin{align*}
qL &= \pi m - 2 \sqrt{\frac{e_{1z}}{e_{2z}}} \arctg \left( \sqrt{\frac{e_{1z}}{e_{2z}}} \right), \\
qL &= \pi m - 2 \sqrt{\frac{e_{1z}}{e_{2z}}} \arctg \left( \sqrt{\frac{e_{1z}}{e_{2z}}} \right),
\end{align*} \]

\( m = 0,1,2,3,... \) (14)

Eqs. (13) and (14) being partial cases of Eq. (12) are identical to equations obtained in [9]. These equations are further simplified for a symmetric heterostructure of crystals of a cubic lattice structure and correspond to the equations in [17].

Interface phonons are described with decaying solutions at both interfaces. Thus, the following inequalities should be valid:

\[ \begin{align*}
\varepsilon_{1z} &> 0, \varepsilon_{11} > 0, \varepsilon_{3z} > 0, \\
\varepsilon_{1z} &< 0, \varepsilon_{2z} < 0.
\end{align*} \] (15)

The potentials \( \Phi_1(z) \) and \( \Phi_3(z) \) are expressed by (9) and (11), while

\[ \Phi_2(z) = A_2 \chi(z) \cos(kz) + B_2 \chi(z) \sin(kz), \]

\[ \chi_z = \frac{e_{1z}}{e_{3z}}. \] (16)

In this case the dispersion relation looks as follows:

\[ \begin{align*}
qL &= 2 \sqrt{\frac{e_{1z}}{e_{2z}}} \arctg \left( \sqrt{\frac{e_{1z}}{e_{2z}}} \right), \\
qL &= 2 \sqrt{\frac{e_{1z}}{e_{2z}}} \arctg \left( \sqrt{\frac{e_{1z}}{e_{2z}}} \right),
\end{align*} \] (17)

Like in the case of confined phonons for the symmetric heterostructure (\( \varepsilon_{1z} = \varepsilon_{3z}, \varepsilon_{11} = \varepsilon_{11} \)) phonon states divide into two types: symmetric (\( \Phi_3(z) = A_2 \cos(kz) \)) and antisymmetric (\( \Phi_3(z) = B_2 \sin(kz) \)). For symmetric confined phonons the dispersion relation looks as

\[ qL = 2 \sqrt{\frac{e_{1z}}{e_{2z}}} \arctg \left( \sqrt{\frac{e_{1z}}{e_{2z}}} \right) + \pi m, \]

\( m = 0,1,2,3,... \) (13)

The dispersion relation of antisymmetric phonons has the form

\[ qL = 2 \sqrt{\frac{e_{1z}}{e_{2z}}} \arctg \left( \sqrt{\frac{e_{1z}}{e_{2z}}} \right) + \pi m, \]

\( m = 0,1,2,3,... \) (18)

and for antisymmetric phonons it can be presented

\[ qL = 2 \sqrt{\frac{e_{1z}}{e_{2z}}} \arctg \left( \sqrt{\frac{e_{1z}}{e_{2z}}} \right) + \pi m. \] (19)

Equations (18) and (19) are reduced to analogous equations in [9], and for cubic crystals to those in [17].
Half-space phonons appear under the condition when polarization waves are decaying inside the nanofilm and oscillating in the half-spaces $|z| \geq L/2$:

$$e_{1i}e_{1z} < 0, \ e_{1i}e_{3z} < 0, \ e_{21}, e_{22} > 0.$$  \hspace{1cm} (20)

In this case it is necessary to consider two types of polarization vibrations:

a) quasi-symmetric:

$$\Phi_1(z) = A_i \cos(\kappa_i z),$$

$$\Phi_2(z) = A_i \sin(\kappa_i z),$$

$$\Phi_3(z) = B_i \cos(\kappa_i z),$$

$$\kappa_i = \sqrt{\frac{e_{11}^{(o)}}{e_{1i}^{(o)}}} q, \ i = 1, 3, \ \chi_2 = \sqrt{\frac{e_{21}^{(o)}}{e_{22}^{(o)}}} q; \hspace{1cm} (21)$$

b) quasi-antisymmetric:

$$\Phi_1(z) = B_i \sin(\kappa_i z),$$

$$\Phi_2(z) = A_i \sinh(\chi_2 z) + B_i \cosh(\chi_2 z),$$

$$\Phi_3(z) = B_i \sin(\kappa_i z).$$  \hspace{1cm} (21')

For first type phonons the dispersion relation is written

$$e_{21} \cos \left( qL \sqrt{\frac{e_{11}}{e_{1i}}} \right) \left( \sqrt{\frac{e_{21}}{e_{22}}} \right) \times$$

$$\times \cosh \left( qL \sqrt{\frac{e_{21}}{e_{22}}} \right) \sin \left( qL \sqrt{\frac{e_{11}}{e_{1i}}} \right) +$$

$$+ e_{21} \cos \left( qL \sqrt{\frac{e_{11}}{e_{1i}}} \right) \sinh \left( qL \sqrt{\frac{e_{11}}{e_{1i}}} \right) +$$

$$+ e_{21} \sqrt{\frac{e_{11}}{e_{1i}}} \sin \left( qL \sqrt{\frac{e_{11}}{e_{1i}}} \right) \times$$

$$\times \sqrt{\frac{e_{22}}{e_{22}}} \cos \left( qL \sqrt{\frac{e_{11}}{e_{1i}}} \right) \cosh \left( qL \sqrt{\frac{e_{11}}{e_{1i}}} \right) +$$

$$+ e_{21} \sqrt{\frac{e_{11}}{e_{1i}}} \sin \left( qL \sqrt{\frac{e_{11}}{e_{1i}}} \right) \sinh \left( qL \sqrt{\frac{e_{11}}{e_{1i}}} \right) = 0.$$  \hspace{1cm} (22)

For second type phonons the dispersion relation is

$$qL = \pi m - 2 \sqrt{\frac{e_{11}}{e_{1i}}} \times$$

$$\times \arctg \left( \sqrt{\frac{e_{21}e_{22}}{e_{21}e_{22}}} \sinh \left( \sqrt{\frac{e_{11}}{e_{22}}} qL \right) \right).$$  \hspace{1cm} (24)

For symmetric phonons and

$$qL = \pi m + 2 \sqrt{\frac{e_{11}}{e_{1i}}} \times$$

$$\times \arctg \left( \sqrt{\frac{e_{21}e_{22}}{e_{21}e_{22}}} \sinh \left( \sqrt{\frac{e_{11}}{e_{22}}} qL \right) \right).$$  \hspace{1cm} (25)

Quasi-antisymmetric phonons are described by the following dispersion relation:

$$e_{1i} \sqrt{\frac{e_{11}}{e_{1i}}} \cos \left( qL \sqrt{\frac{e_{11}}{e_{1i}}} \right) \left( \sqrt{\frac{e_{11}}{e_{1i}}} \right) \times$$

$$\times \cosh \left( qL \sqrt{\frac{e_{11}}{e_{1i}}} \right) \sin \left( qL \sqrt{\frac{e_{11}}{e_{1i}}} \right) -$$

$$- e_{1i} \sqrt{\frac{e_{11}}{e_{1i}}} \cos \left( qL \sqrt{\frac{e_{11}}{e_{1i}}} \right) \sin \left( qL \sqrt{\frac{e_{11}}{e_{1i}}} \right) +$$

$$+ e_{21} \sqrt{\frac{e_{11}}{e_{1i}}} \sin \left( qL \sqrt{\frac{e_{11}}{e_{1i}}} \right) \cosh \left( qL \sqrt{\frac{e_{11}}{e_{1i}}} \right) -$$

$$- e_{21} \sqrt{\frac{e_{11}}{e_{1i}}} \sin \left( qL \sqrt{\frac{e_{11}}{e_{1i}}} \right) \sinh \left( qL \sqrt{\frac{e_{11}}{e_{1i}}} \right) = 0.$$  \hspace{1cm} (23)
cause of absence of decaying the potential \( \Phi(\vec{r}) \) is different from zero even for \( |z| = \infty \). One should use additional conditions to obtain the dispersion relation of these phonons. It can be proved [1] that without regard for delaying effects for propagating waves the wave vector and the electric field vector are co-linear (\( \vec{Q} \times \vec{E} = 0 \)):

\[
Q_i \frac{\partial \Phi(\vec{r})}{\partial \rho} - q \frac{\partial \Phi(\vec{r})}{\partial z} = 0.
\]

On the basis of this equation one can get the conditions at the interfaces

\[
\begin{align*}
\left[ \frac{e_{22}(\omega)}{e_{21}(\omega)} \right] \frac{\partial \Phi_2(z)}{\partial z} & \bigg|_{z=-L/2} \left[ \frac{e_{11}(\omega)}{e_{21}(\omega)} \right] \frac{\partial \Phi_1(z)}{\partial z} \bigg|_{z=-L/2}, \\
\end{align*}
\]

For symmetric three-layer heterosystem \( (\kappa_i = \kappa_1) \) there are two types of propagating phonons: symmetric —

\[
\Phi_i(z) = A_i \cos(\kappa_i z),
\]

\[
\Phi_2(z) = A_2 \cos(\kappa_i z) + B_2 \sin(\kappa_i z),
\]

\[
\Phi_3(z) = A_3 \cos(\kappa_i z)
\]

and antisymmetric —

\[
\Phi_1(z) = B_1' \sin(\kappa_i z),
\]

\[
\Phi_2(z) = A_2' \cos(\kappa_i z) + B_2' \sin(\kappa_i z),
\]

\[
\Phi_3(z) = B_3' \sin(\kappa_i z).
\]

By taking account of conditions at the interfaces one can get the dispersion relations for symmetric and antisymmetric phonons. There is a non-dispersive phonon mode the frequency of which is determined by the equation

\[
e_{12} \sqrt{e_{22} - e_{21}} = 0.
\]

And also the dispersion relation is

\[
qL = \pi \frac{e_{12}}{\sqrt{e_{21} e_{11}}} m,
\]

where \( m = 2, 4, 6, \ldots \) is for symmetric, and \( m = 1, 3, 5, \ldots \) is for asymmetric phonons. Equations (31) and (32) are identical to those obtained in [9]. As shown above, this phonon type does not exist in every heterosystem. In heterosystems of cubic crystals these phonons do not appear. Only if heterosystem crystals are of hexagonal lattice structure, then Eqs. (28), (31), (32) describing these phonons can have solutions when the required conditions concerning dielectric functions are satisfied.

In order to research polaron states we consider the Hamiltonian of the phonon system interacting with an electron:

\[
\hat{H} = \hat{H}_e + \hat{H}_{ph} + \hat{H}_{int}.
\]

In the effective mass approximation \( \hat{H}_e \) for one-axis crystal has the form

\[
\hat{H}_e = -\frac{\hbar^2}{2m_\perp} \nabla^2 - \frac{\hbar^2}{2m_\parallel} \frac{\partial^2}{\partial z^2} + V,
\]

where \( m_\perp \) and \( m_\parallel \) are electron effective masses in the perpendicular and parallel directions to the \( C \) — axis, \( V \) is the electron potential energy. For a bulk crystal \( V = 0 \).
The phonon energy operator in the occupation number representation is written

\[ \hat{H}_{ph} = \sum_{\nu} \hbar \omega_{\nu} (b_{\nu}^\dagger b_{\nu} + \frac{1}{2}) , \]  

(35)

where \( b_{\nu}^\dagger \) is a phonon birth operator with the wave vector \( \tilde{Q} \) of the phonon mode \( \nu \).

Polarization phonon frequency \( \omega \) is found from dispersion relation (5). For the wurtzites under consideration conditions \[9\] are fulfilled:

\[ \omega - \omega_{lz} < \omega - \omega_{lt} < \omega - \omega_{lz} \]  

(36)

If we account for \( Q \) and \( \sin \theta \) and \( \cos \theta \), then from Eq. (5) under conditions (36) we can get two solutions for \( \omega \):

\[ \omega_1 = \omega_{lz} \sin^2 \theta + \omega_{lt} \sin^2 \theta , \]

(37)

\[ \omega_2 = \omega_{lz} \sin^2 \theta + \omega_{lt} \cos^2 \theta . \]

(38)

The first solution can be referred to as frequency of mainly longitudinal modes, while the second one as frequency of mainly transverse modes. The electron-phonon interaction operator for a bulk crystal can be given by \[7, 9\]

\[ \hat{V}_{IF} = \sum_{\nu} \left( V^{(1)}(Q) e^{iQz} (b_{\nu} + b_{\nu}^\dagger) \right) \]  

(39)

where \( V^{(1)}(Q) \) is the phonon wave vector:

\[ \sqrt{S} LQ \frac{\alpha(\omega) \sin^2 \theta + \epsilon(z) \cos^2 \theta}{\chi(\omega) \chi(z)} , \]

\[ \left( 4 \pi \hbar e^2 \right)^{\frac{1}{2}} \alpha(\omega)^2 + \chi(z)^2 . \]

\( S \) is the crystal volume, the derivative over frequency is taken at the point \( \omega = \omega_{l} \).

It easy to make sure that in the case

\[ \omega_{lz} = \omega_{lt} , \]

(40)

\[ \epsilon_{lz}^x = \epsilon_{lt}^x \]

(41)

equations (37)-(39) transfer to the well-known formulas for a cubic lattice structure crystal [18, 19].

For a hexagonal symmetry heterostructure in which two semi-infinite crystals are adjacent to a nanofilm (double heterosystem), there exist four types of optical phonon modes. These modes are referred to — like those for heterosystems of zinc blende — based crystals — interface, confined, half-space. Moreover, generally speaking, there can be a new phonon type in the system (compared to heterostructures of cubic lattice structure crystals) i.e., phonons that propagate in the medium (propagating phonons). Analogously to the case of cubic lattice structure crystal heterosystem, the operator of the electron interaction with different modes can be represented as a sum of symmetric and antisymmetric parts, that is for all the mentioned types there also exist symmetric and antisymmetric phonons.

In general, the electron-phonon interaction operator is a sum of eight terms, each of them is given by

\[ \hat{V} = \sum_{\nu} V(\tilde{q}) e^{i\tilde{q} \cdot \tilde{r}} (b_{\nu} + b_{\nu}^\dagger) , \]

(42)

where \( \tilde{q} \) is the phonon wave vector : \( \tilde{q} = (q_x, q_y) \).

The function \( V(\tilde{q}) \) determines the phonon type with which an electron interacts. For interface symmetric or antisymmetric phonons \( V(\tilde{q}) \) is expressed by

\[ \left[ \frac{S}{2} \right]^{\frac{1}{2}} \left[ \begin{array}{c} \epsilon_{c1} \left( \frac{q_L}{2} \right) \\
\epsilon_{c2} \left( \frac{q_L}{2} \right) \end{array} \right] \times \left[ \begin{array}{c} \epsilon_{c1} \left( \frac{q_L}{2} \right) \\
\epsilon_{c2} \left( \frac{q_L}{2} \right) \end{array} \right] \]

(43)

The frequencies of symmetric (antisymmetric) phonons are determined from the dispersion relations:

\[ \epsilon_{c1} \left( \frac{q_L}{2} \right) - \epsilon_{c2} = 0 \]

(44)

within the frequency region when the inequalities are valid

\[ \epsilon_{c1} \left( \omega \right) < 0 , \epsilon_{c2} \left( \omega \right) > 0 \]

and

\[ i \epsilon_{c1} \left( \omega \right) \epsilon_{c2} \left( \omega \right) > 0 . \]

In formulas (43), (44) the following notation is introduced:
For the confined phonons (symmetric and antisymmetric) \( V(q) \) is

\[
V^{[S]}_c(q) = \frac{V^{[S]}_c(q) \cdot V^{[S]}_c(q, z)}{C} = \frac{1}{\sqrt{S}} \frac{\partial}{\partial \omega} \left( e_{1z} q^2 + e_{1z} k_m^2 \right) - 2q f_s(\omega) \cos \left( \frac{k_m L}{2} \right) \left\{ \begin{array}{l}
\cos (k_m z) \\
\sin (k_m z)
\end{array} \right\}, \quad \left| \omega \right| < \frac{L}{2}
\]

(45)

where

\[
\left\{ \begin{array}{l}
f_s(\omega) \\
f_s(\omega)
\end{array} \right\} = \text{sgn}(e_{1z}) \sqrt{-e_{1z} (\omega) e_{1z} (\omega)} \times
\left\{ \begin{array}{l}
\sin \left( \frac{k_m L}{2} \right) \\
\cos \left( \frac{k_m L}{2} \right)
\end{array} \right\} - \text{sgn}(e_{1z}) e_{1z} \left\{ \begin{array}{l}
\cos \left( \frac{k_m L}{2} \right) \\
\sin \left( \frac{k_m L}{2} \right)
\end{array} \right\}
\]

(46)

\( k_m \) is determined from

\[
e_{1z} k_m \left\{ \begin{array}{l}
\sin \left( \frac{k_m L}{2} \right) \\
\cos \left( \frac{k_m L}{2} \right)
\end{array} \right\} - e_{2z} k_2 \left\{ \begin{array}{l}
\cos \left( \frac{k_m L}{2} \right) \\
\sin \left( \frac{k_m L}{2} \right)
\end{array} \right\} = 0,
\]

under the condition that

\[
\pi \frac{2m}{L} < k_m < \pi \frac{2m+2}{L}.
\]

For the symmetric phonons (\( m = 0,1,2,\ldots \)) and for antisymmetric phonons (\( m = 1,2,3,\ldots \)).

The semi-confined polarization phonons — their \( E_s \) and \( D_s \), being continuous functions at either interface with the properties similar to those of bulk crystal phonons — if \( z = \pm \infty \), are characterized by the following \( V(Q) \) for the symmetric, antisymmetric phonon modes:

\[
V^{[S]}_s(q) = \frac{V^{[S]}_s(q) \cdot V^{[S]}_s(q, z)}{C} = \frac{1}{\sqrt{S}} \frac{\partial}{\partial \omega} \left( e_{1z} q^2 + e_{1z} k_m^2 \right) - 2q f_s(\omega) \cos \left( \frac{k_m L}{2} \right) \left\{ \begin{array}{l}
\cos (k_m z) \\
\sin (k_m z)
\end{array} \right\}, \quad \left| \omega \right| < \frac{L}{2}
\]

(47)

\( e_{1z} k_m \left\{ \begin{array}{l}
\sin \left( \frac{k_m L}{2} \right) \\
\cos \left( \frac{k_m L}{2} \right)
\end{array} \right\} - e_{2z} k_2 \left\{ \begin{array}{l}
\cos \left( \frac{k_m L}{2} \right) \\
\sin \left( \frac{k_m L}{2} \right)
\end{array} \right\} = 0,
\]

The electron potential energy in the heterosystem is chosen as a rectangular potential well.
Then the wave function looks as follows:

\[ \psi_e (\vec{r}) = \frac{1}{\sqrt{S}} e^{i \vec{k} \cdot \vec{r}} \phi_n (z) , \]

where \( \phi_n (z) = \begin{cases} \alpha \sin (zL) + \beta \cos (zL) , & |z| < L/2 , \\ Be^{-\chi_0 z} , & |z| > L/2 . \end{cases} \)

and the electron energy is described by

\[ E_n (k) = \frac{p^2}{2m} + \tilde{E}_n , \]

\( \tilde{p} \) is the electron impulse, and \( \tilde{E}_n \) is found from the dispersion relation which is a result of continuity condition of the wave function and its probability current density at the interfaces.

To determine the polaron energy, the perturbation theory and the variational Lee-Low-Pains (LLP) method are used [19, 20]. By applying the LLP method, it is taken into account that the considered system contains a fast and a slow subsystems. The electron motion in the direction normal to the interface is assumed a fast subsystem. The adiabatic approximation is therefore used, Hamiltonian (33) is averaged over the functions of the electron ground stationary state in the motion along the z-axis:

\[ \hat{H}_{\text{ef}} = \langle \varphi_1 (z) \rangle \hat{H} \varphi_1 (z) \rangle = \]

\[ = \tilde{E}_1 + \frac{p^2}{2m} + \hat{H}_{\text{ph}} + \sum q \langle \tilde{\varphi} (\tilde{q}) \rangle \hat{b}_q \hat{b}_q + \text{e.c.} , \]

where \( M_{1n} = \int_0^\infty \varphi_1^* (z) \psi (z) \varphi_n (z) dz , \ n = 1 . \)

Two unitary transformations are consecutively applied to Hamiltonian (20) by the operators

\[ \hat{S} = \exp \left[ \frac{i}{\hbar} \int \left( \tilde{p} - \sum_{\tilde{q}} \tilde{b}^+_{\tilde{q}} \tilde{b}_{\tilde{q}} \tilde{q} \right) \right] , \]

\[ \hat{U} = \exp \left[ \sum q \langle \tilde{b}^+_{\tilde{q}} f (\tilde{q}) - \tilde{b}_{\tilde{q}} f^* (\tilde{q}) \rangle \right] , \]

where \( \tilde{p} = \hbar \tilde{k} \) is the polaron impulse.

After averaging the obtained expression over the vacuum phonon state and minimizing the functional over \( f (\tilde{q}) \) and \( f^* (\tilde{q}) \), the polaron energy of the heterosystem is found [21-23]:

\[ E_{\text{pol}} (k) = \overline{E}_1 + \frac{h^2 k^2}{2m} \left( 1 + \eta^2 \right) + \]

\[ -2 \sum q \frac{\langle \tilde{\varphi} (\tilde{q}) \rangle^2 |M_{11}|^2}{h_0 - \tilde{h} \tilde{\varphi} \tilde{\varphi} + \frac{h^2 q^2}{2m}} + \]

\[ + \sum q \frac{\langle \tilde{\varphi} (\tilde{q}) \rangle^2 |M_{11}|^2}{h_0 - \tilde{h} \tilde{\varphi} \tilde{\varphi} + \frac{h^2 q^2}{2m}} , \]

(52)

where \( \eta \tilde{p} = \sum \int \frac{\langle \tilde{\varphi} (\tilde{q}) \rangle^2}{h \tilde{q}} \).

\[ f_{\text{min}} (\tilde{q}) = \frac{V_{11} \langle \tilde{\varphi} (\tilde{q}) \rangle M_{11}^*}{h_0 + \frac{h^2 q^2}{2m} - \frac{h^2 \tilde{k} \tilde{q}(1-\eta)}{2m}} . \]

The polaron energy in the bulk material is determined by similar formulas [19]. The difference is that expression (52) contains the function \( M_{11} \), resulting from the translational symmetry deviation of the system in the z-direction.

The crystals \( \text{AlN} , \text{GaN} \) are characterized by a small constant of the electron-phonon interaction \( (\alpha = 0.681 , \alpha = 0.466 \) accordingly), therefore to determine the polaron energy, one can use the perturbation theory [24, 25]:

\[ E_{\text{pol}} (k) = \overline{E}_1 + \frac{h^2 k^2}{2m} + \]

\[ + \sum \frac{\langle \tilde{\varphi} (\tilde{q}) \rangle^2 |M_{11}|^2}{h_0 - \tilde{h} \tilde{\varphi} \tilde{\varphi} + \frac{h^2 q^2}{2m}} , \]

(53)

In receiving formula (53), the adiabatic approach was not used, thus it can be applied not only for small values \( L \) of quantum well widths. Expressions (52) and (53) reflect the wave-vector dependence of the polaron energy — the quasiparticle dispersion relation.
2. Discussion of the results

The specific calculations are performed for the heterostructures AlN/GaN/AlN, AlN/GaN/AlN, GaN/ZnO/AlN. Material parameters are taken to be: $\varepsilon^c = 5.29$, $\omega_{li} = 743 \text{ sm}^{-1}$, $\omega_{lz} = 735 \text{ sm}^{-1}$, $\omega_{lz} = 561 \text{ sm}^{-1}$, $\omega_{lt} = 533 \text{ sm}^{-1}$ for GaN; $\varepsilon^v = 4.68$, $\omega_{lv} = 916 \text{ sm}^{-1}$, $\omega_{lp} = 893 \text{ sm}^{-1}$, $\omega_{lt} = 673 \text{ sm}^{-1}$, $\omega_{ltz} = 660 \text{ sm}^{-1}$ for AlN; $\varepsilon^G = 3.7$, $\omega_{lt} = 578 \text{ sm}^{-1}$, $\omega_{lz} = 594 \text{ sm}^{-1}$, $\omega_{lt} = 381 \text{ sm}^{-1}$, $\omega_{lt} = 409 \text{ sm}^{-1}$ for ZnO [7]. Unlike the case of heterostructures of isotropic crystals, there appears a number of peculiarities of optical phonon spectrum. The main reason of this result is found in dispersion relation (5) from which, generally speaking, one cannot separate the wave vector of vibration frequency. In addition, if we take account of the conditions at the interfaces, we obtain finite energy integrals for different mode phonons. By comparing theory and experiment, these regions of phonon frequencies make it possible to determine composition of the nanoheterostructure.

Fig. 2. The dispersion relation of polarization optical phonons in a quantum well AlN/GaN/AlN. Confined (1), interface (2) and half-space (3) phonon modes in the given intervals of phonon frequencies are presented. Characteristic frequencies are indicated with dashed curves.

Fig.2 presents the dispersion relations of confined, interface and half-space polarization phonons. It is seen that every phonon mode exists in two frequency regions. For confined phonons of the heterostructure AlN/GaN/AlN frequency intervals are: $\omega_{lz} \leq \omega_i \leq \omega_{ltz}$, $\omega_{lz} \leq \omega_{h} \leq \omega_{lz}$. Interface phonons exist at the frequencies: $\omega_{lt} \leq \omega_i \leq \omega_{ltz}$, $\omega_{lz} \leq \omega_{h} \leq \omega_{lz}$, and half-space phonons — $\omega_{lz} \leq \omega_{h} \leq \omega_{lz}$, $\omega_{lt} \leq \omega_{h} \leq \omega_{lz}$. Unlike in heterostructures of cubic lattice structure crystals the frequency of confined phonons is not constant, it is a monotonous function of the wave vector and also depends on the number $m$. In particular, in the region $\omega_i$ the least value of $m$ ($m = 0$ for antisymmetric modes) is related to the mode with the smallest, and in the region $\omega_i$ with the largest frequency. At the given wave vector the rise of $m$ results in the reduction (interval $\omega_i$) or in the increase (interval $\omega_i$) of frequency. There are four interface phonon modes in two regions of frequencies. For small values of the wave vector they sufficiently differ in frequency. The increase of $qL$ results in the fact that two modes in pairs degenerate into one also at great values of $qL$. Similar dependences are received for half-space phonons.

The data of calculations of the confined and interface phonon spectrum of asymmetric nanoheterostructures vacuum/GaN/AlN, GaN/ZnO/AlN are given in Fig. 3(a,b). Because of more rigid conditions applied on the existence of interface phonons, the number of these phonon modes decreases compared with a symmetric heterosystem. Alongside, the degeneracy of the spectrum is lifted at large values of the wave vector. As to confined phonons, the heterosystems differ not only in frequency numerical values but also in the dependence $\omega = \omega(q)$. For both frequency intervals the dispersion relations of confined phonons of the heterosystem vacuum/GaN/AlN are qualitatively identical to those of the structure AlN/GaN/AlN. In the heterostructure GaN/ZnO/AlN these dependences are slightly different: the rise of $qL$ is followed by the increase of frequencies for “lower” interval, and by their decrease for “upper” frequency region. The analysis of existence conditions of propagating phonons shows that in the heterosystems under consideration they do not exist.

In the investigation of polaron states, we consider the region of small values of wave vectors ($k \approx 0$). The quantities $\eta(k)$ and $E_{pol}(k)$ are obtained by expanding the corresponding expressions in series and restricting to first terms of the expansion [19]. Regarding the polaron dispersion relation in a small but finite region of the wave-vector change $0 \leq \eta < k_f$, $k_f = \sqrt{\frac{2m_{\varepsilon}^{\omega}}{h}} \ll k_0$, where $k_0$ is the wave vector critical value in the Brillouin zone, the calculations $E_{pol} = E_{pol}(k)$ in this report have been carried out without any additional simplification of formulas (52), (53).
that they have little effect on the polaron binding energy. For illustration, at $L = 25\,\text{Å}$ for the AlN/GaN/AlN double heterostructure within the infinite quantum well (IQW) model, the contribution makes 22.536 meV in the case of confined phonons, for interface phonons 22.633 meV, and half-space phonons 2.035 meV, while at $L = 100\,\text{Å}$ it is 32.484 meV, 8.711 meV, 1.184 meV respectively. The comparison of two models — the IQW ($V = \infty$ in (49)) and the finite quantum well (FQW) at the interface of the heterosystem — shows similar results for all phonon types not only for great $L$ because of significant real quantum well depth. The difference becomes essential (particularly for the confined phonons at $L < 60\,\text{Å}$ (e.g., if $L = 50\,\text{Å}$, it makes 17%)).

Fig. 3. The dispersion relation of polarization optical phonons in quantum wells GaN/ZnO/AlN (a) and vacuum/GaN/AlN (b): confined (1) and interface (2) phonon modes in the given intervals of phonon frequencies. Characteristic frequencies are indicated with dotted curves.

In Fig.4 the dependence of the polaron binding energy of the heterosystem AlN/GaN/AlN on the nanofilm thickness is presented. For the comparison the polaron binding energies of bulk crystals GaN and AlN are given. It is seen that the polaron binding energy ($E_c = E_{pol}(0)$) in a bulk crystal GaN is smaller than that in the heterosystem. The reduction of quantum well width ($L$) leads to the increase of this energy and the rise of the dispersion relation deformation.

As to partial contributions, the confined phonons are predominant at $L > 40\,\text{Å}$, though one cannot neglect interface phonon contributions in the range of $40\,\text{Å} < L < 100\,\text{Å}$. For thicknesses $L < 30\,\text{Å}$ the interface phonon contribution becomes greater than that of the confined phonons. As to the half-space phonon contribution, the calculations show

Fig.4. The polaron binding energy of the bulk crystals GaN (7), AlN (8) and heterosystem AlN/GaN/AlN in case of IQW (curves 1, 3, 5), FQW (curves 2, 4, 6). 1, 2 — confined phonons are taken into account, 3, 4 — interface phonons are regarded, 5, 6 — all phonons are taken into account.

Fig.5 shows the dependence of the dispersion relation of a polaron that moves parallel to the heterosystem interfaces at $L = 25\,\text{Å}$. In the range of small wave-vector values for all phonon modes and both potential well models, the quadratic dependences of functions $E_{pol} = E_{pol}(k)$ are received. The wave-vector value rise results in the “dispersion relation deformation”. If one takes account of all phonon modes, as is seen from the figure, the polaron energy for the $V = \infty$ model is smaller than that for the finite value of $V$. However, the wave-vector growth is followed by the reduction of the polaron energy difference within different QW models.
Fig. 5. Polaron energy of the heterosystem AlN/GaN/AlN for QW at $L = 25\,\text{Å}$ in the cases of IQW (curves 1, 3, 5) and FQW (curves 2, 4, 6). 1, 2 show the energy with regard for confined phonons, 3, 4 stand for the interface phonons, 5, 6 indicate all phonons.

Since the dispersion relation is known, one can determine the polaron average speed:

$$\bar{v} = \frac{1}{\hbar} \nabla \cdot E_{\text{pol}}(\vec{k}) .$$

This quantity enters the formulas of kinetic coefficients as well as defines the degree of polaron dispersion relation “deformation”. It is seen from Fig. 6 that in the region of large wave-vector values $k \approx k_f$, the increase of $k$ — as a result of all phonon modes contribution — leads to $v = v(k)$ approaching saturation, i.e., the polaron dispersion relation $E_{\text{pol}} = E_{\text{pol}}(k)$ transfers from a quadratic function (at $k = 0$) into a liner one (at $k = k_f$).

Alongside with the speed, the polaron effective mass is also important:

$$\frac{1}{m_p} = \frac{\hbar^2}{c k_f^2} \frac{\partial^2 E_{\text{pol}}(k)}{\partial k^2} .$$

Fig. 7 shows that the reduction of $L$ is followed by polaron effective mass growth. It points out — similarly to the polaron binding energy enhancement — the increase of the effective electron-phonon interaction. The rise of particle spatial confinement also leads to its effective mass growth.

Therefore, the article presents wave vector —dependent energies of confined, interface, half-space, and propagating phonons for symmetric and asymmetric three-layer nanoheterosystems of hexagonal lattice structure crystals. The specific calculations are performed for three-layers symmetric ($\text{AlN/GaN/AlN}$), and three-layer asymmetric heterosystems ($\text{vacuum/GaN/AlN}$, $\text{GaN/ZnO/AlN}$). It is defined and analysed the character of frequency dependences of every phonon mode type as a function of wave vector. The report also presents a theoretical study of the polaron dispersion relation in the GaN crystal and $\text{AlN/GaN/AlN}$ double nanoheterostructure by taking into account all types of polarization oscillations with which an electron interacts within the models of infinite and finite barriers. Calculations of the average speed and polaron effective mass are performed. It is shown that, the interface phonon contribution in the polaron energy decreases with nanofilm thickness increase, while that of the confined phonons grows. The calculation data of the polaron dispersion relation in the region $k < k_f$ in
different directions of the polaron wave vector with respect to the C-axis of the crystal are given. The reduction of the dimension number of the system, increase of the wave-vector \( k \) cause an effective enhancement of the electron-phonon interaction.

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