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Electronic polaron of the AlN/GaN/AlN double nanoheterostructure of hexagonal symmetry crystals

V. I. BOICHUK, V. A. BORUSEVYCH*, I. S. SHEVCHUK
Department of Theoretical Physics, Ivan Franko Drohobych State Pedagogical University,
24 Ivan Franko Str., Drohobych 82100, Ukraine

A theoretical study of the polaron dispersion relation in the *GaN* crystal and *AlN/GaN/AlN* double nanoheterostructure is presented. Every type of polarization oscillation with which an electron interacts is taken into account. Calculations are performed in the framework of an infinite and a finite band gap models. It is shown that with the nanofilm thickness increase, a contribution of the interface phonon in the polaron energy decreases, while that of the confined phonons gains in value. The calculation results of the polaron dispersion relation in the region of $k < k_f$ in different polaron wave-vector directions with respect to the *c*-axis of the crystal are given. Also, the polaron average speed and effective mass are calculated. The results suggest an effective enhancement of the electron-phonon interaction with lowering of the system dimensions number.

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1. Introduction

In recent years quantum heterostructures formed by III-V nitrides (GaN, AlN, InN) have attracted particular attention because of their potential applications in optoelectronics [1-5].

In particular, progress in growth technology of quantum dot structures based on crystals with hexagonal symmetry made it possible to fabricate photodetectors and lasers that function due to intersubband transitions. The electron-phonon interaction in such processes plays an important role.

Moreover, they are also interesting from purely physical point of view since wurtzite-based crystals have lower symmetry compared to zinc-blende counterparts which are much more extensively studied. Crystals of both symmetry types differ not only in the electron and hole spectra but also in the phonon spectrum, and the phonon-quasiparticle interaction [6-8].

Over the past decade numerous theoretical and experimental studies on polarization and acoustic phonons as well as the electron-phonon interaction in wurtzite semiconductor heterostructures have been reported [8-13]. Most efforts have been directed toward a thorough investigation of the phonon spectra in single heterointerface systems [6-9], as well as the phonon dispersion in superlattice structures within the dielectric continuum approach and the Loudon uniaxial model [12, 13].

The authors have obtained the dispersion relations to describe every type of polarization phonons, have drawn and analysed the plots of these phonon dispersion dependences. They also have presented general Hamiltonians of an electron interacting with different phonon modes.

However, the polaron states in the heterointerface systems based on wurtzite structure crystals have not been sufficiently investigated [14-15]. Most attempts in this direction are restricted to research of the polaron states in bulk crystals.

The present report is focused on a theoretical study of the polaron dispersion relation in the GaN crystal and the AlN/GaN/AlN double heterointerface nanoscale structure.

2. Statement of the problem

A bulk ideal wurtzite crystal with a unit-cell as a hexagonal prism is considered. The III-V nitrides belong to C_{6v}^{4} group of symmetry. They are formed by two mutually penetrable hexagonal-packed sublattices which are shifted along the C-axis (axis OZ of the coordinates system) by 5/8 of the lattice constant. A unit cell contains four atoms. Therefore, there exist nine optical and three acoustic modes. But only two regions of optical phonons are active in the infrared range and during combination dispersion. They correspond to the unreducable representations A_1 and E_1 of wave-vector group at the $\tilde{A}$ point of the Brillouin zone. A_1 and E_1 modes split into LO and TO components.

Due to optical anisotropy of such crystals long wavelength optical vibrations can be classified with respect to the C-axis orientation, phonon wave vector $\vec{\mathrm{Q}}$, electric field $\vec{E}$ and polarization $\vec{P}$. This classification makes it possible to divide them into the so-called ordinary and extraordinary optical phonons. The ordinary phonons with E_1-symmetry are always transversal (both $\vec{E}$ and $\vec{P}$ are perpendicular to $\vec{\mathrm{Q}}$ and the C-axis simultaneously) and polarized in the plane that is perpendicular to the vector $\vec{\mathrm{Q}}$. The frequency of the ordinary phonons does not depend on the angle θ between the vector $\vec{\mathrm{Q}}$ and C-axis. The extraordinary phonons are related to z- and $\perp$-polarized vibrations. The mode polarized in the direction of the OZ-axis has A_1-symmetry, and the one $\perp$-polarized has E_1-symmetry. If the angle θ equals zero, one oscillation is A_1 (LO)-phonon, and the other is E_1 (TO)-phonon. If θ changes from 0 to $\pi/2$, these modes become gradually A_1 (TO)- and E_1 (LO)-phonons with neither a distinct feature of LO- or TO-character nor A_1- or E_1-symmetry. Thus, in the case of $\theta \neq 0$ and $\theta \neq \pi/2$ the extraordinary vibrations are a combination of LO and TO modes.

The extraordinary phonon dispersion relation in a long-wavelength region is given by

$$\varepsilon_\perp(\omega) q_\perp^2 + \varepsilon_z(\omega) \mathrm{Q}_z^2 = 0, \tag{1}$$

where, $\varepsilon_\perp(\omega) = \varepsilon_\perp^\infty \dfrac{\omega^2 - \omega_{\perp L}^2}{\omega^2 - \omega_{\perp T}^2}$, $\varepsilon_z(\omega) = \varepsilon_z^\infty \dfrac{\omega^2 - \omega_{zL}^2}{\omega^2 - \omega_{zT}^2}$, $\varepsilon_\perp^\infty$, ε_z^∞ are high-frequency dielectric permittivities, $\omega_{\perp L}$ and ω_{zL} are long-wavelength E_1 (LO)- and A_1 (LO)-phonon frequencies, $\omega_{\perp T}$ and ω_{zT} are transversal E_1 (TO) and A_1 (TO)-phonons at $\vec{\mathrm{Q}}=0$.

The Hamiltonian of the phonons system interacting with an electron is considered to study the polaron states:

$$\hat{\mathrm{H}} = \hat{\mathrm{H}}_{\mathrm{e}} + \hat{\mathrm{H}}_{\mathrm{ph}} + \hat{\mathrm{H}}_{\mathrm{int}}. \tag{2}$$

In the effective mass approximation, $\hat{\mathrm{H}}_{\mathrm{e}}$ for a uniaxial crystal is represented through

$$\hat{\mathrm{H}}_{\mathrm{e}} = -\frac{\hbar^2}{2m_\perp}\nabla_{\vec\rho}^2 - \frac{\hbar^2}{2m_{||}}\frac{\partial^2}{\partial z^2} + V,\ \ \nabla_\rho^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}, \tag{3}$$

where $m_\perp$ and $m_{||}$ are effective masses of an electron in the directions perpendicular and parallel to the C-axis respectively, V is the potential energy of an electron. In the bulk case, $V = 0$.

The phonon energy operator in the representation of occupation numbers takes the form

$$\hat{H}_{ph} = \sum_{\vec{\mathrm{Q}},\nu} \hbar\omega_\nu(\vec{q})\left(b_{\vec{\mathrm{Q}},\nu}^{+} b_{\vec{\mathrm{Q}},\nu} + 1/2\right), \tag{4}$$

where $b_{\vec{\mathrm{Q}},\nu}^{+}$ is the creation operator with the wave vector $\vec{\mathrm{Q}}$ of phonon mode ν.

The frequency of polarizations ω is obtained from Eq. (1). For the wurtzites considered in the present paper, conditions are fulfilled [7]:

$$\begin{aligned} &\left|\omega_{\perp,L} - \omega_{z,L}\right|, \left|\omega_{\perp,T} - \omega_{z,T}\right| << \\ &<< \left|\omega_{\perp,L} - \omega_{\perp,T}\right|, \left|\omega_{z,L} - \omega_{z,T}\right|. \end{aligned} \tag{5}$$

By taking into account that $q = \mathrm{Q}\cdot\sin(\theta)$, and $\mathrm{Q}_z = \mathrm{Q}\cdot\cos(\theta)$, from Eq. (1) with regard for condition (5), the solutions are

$$\omega_l^2 = \omega_{z,L}^2 \cos^2\theta + \omega_{\perp,L}^2 \sin^2\theta, \tag{6}$$

$$\omega_t^2 = \omega_{z,T}^2 \sin^2\theta + \omega_{\perp,T}^2 \cos^2\theta, \tag{7}$$

These are predominantly longitudinal and transverse modes, respectively. The electron – optical-phonon Hamiltonian for the bulk material can be given as [6, 7]

$$\hat{H}_{\mathrm{int}} = \sum_{\vec{\mathrm{Q}}} V^{(1)}(\vec{\mathrm{Q}})\cdot V^{(2)}(\vec{\mathrm{Q}},z) e^{i\vec{q}\vec{\rho}}\left(b_{\vec{\mathrm{Q}}} + b_{-\vec{\mathrm{Q}}}^{+}\right), \tag{8}$$

where $V^{(1)} = \dfrac{C}{\sqrt{S\tilde{L}}\mathrm{Q}} \dfrac{1}{\sqrt{\dfrac{\partial}{\partial\omega}\left(\varepsilon_\perp(\omega)\sin^2\theta + \varepsilon_z(\omega)\cos^2\theta\right)}}$,

$V^{(2)}(\vec{\mathrm{Q}},z) = e^{i\mathrm{Q}_z z}$,

$$C = \left(4\pi\hbar e^2\right)^{1/2},\ \ \mathrm{Q}^2 = q^2 + \mathrm{Q}_z^2,$$

$S\tilde{L}$ is the crystal volume, the derivative with respect to frequency is taken at a point $\omega = \omega_l$.

It is easy to see that in the case of

$$\omega_{\perp,L} = \omega_{z,L},\ \ \omega_{\perp,T} = \omega_{z,T}, \tag{9}$$

$$\varepsilon_\perp^\infty = \varepsilon_z^\infty \tag{10}$$

Eqs. (6)-(8) are transformed into the well-known formulas for the crystal with cubic symmetry [16, 17].

For hexagonal symmetry heterostructures with a nanofilm adjacent at either side to two semi-infinite crystals (double heterointerface nanoscale system), there exist four different types of optical phonon modes. These modes are referred to, similarly to those of zinc-blende-based heterosystem crystals, as interface, confined and semiconfined. Moreover, generally speaking, there can be a new phonon type in the system (compared to heterostructures of cubic symmetry crystals) i.e., phonons that propagate in the medium (propagating phonons). Analogous to the case of cubic symmetry 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 a general case, the electron-phonon interaction operator is a sum of eight terms each of them assumes the form

$$\hat{H} = \sum_{\vec{q}} V(\vec{q}) e^{i\vec{q}\vec{\rho}} \left(b_{\vec{q}} + b^{+}_{-\vec{q}} \right), \tag{11}$$

where $\vec{q}$ is the phonon wave vector $\vec{q}(q_x, q_y)$.

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

$$V_{IF}^{\left\{ \begin{smallmatrix} S \\ A \end{smallmatrix} \right\}}(\vec{q}) = V_{IF}^{(1)}(\vec{q}) \cdot V_{IF}^{(2)}(\vec{q}, z) =$$

$$= \frac{C}{\sqrt{S}} \left[2q \left| \frac{\partial}{\partial \omega} \left(\varepsilon_{c1} \left\{ \begin{matrix} th\left(\varepsilon_{b1} \dfrac{qL}{2} \right) \\ cth\left(\varepsilon_{b1} \dfrac{qL}{2} \right) \end{matrix} \right\} - \varepsilon_{c2} \right) \right| \right]^{-1/2} \times$$

$$\times \left\{ \begin{matrix} \left\{ \begin{matrix} ch\left(\varepsilon_{b1} qz \right) \Big/ ch\left(\varepsilon_{b1} \dfrac{qL}{2} \right) \\ sh\left(\varepsilon_{b1} qz \right) \Big/ sh\left(\varepsilon_{b1} \dfrac{qL}{2} \right) \end{matrix} \right\}, \quad |z| \le \dfrac{L}{2} \\ \left\{ \begin{matrix} 1 \\ \operatorname{sgn}(z) \end{matrix} \right\} \exp\left[-\varepsilon_{b2} q \left(|z| - \dfrac{L}{2} \right) \right], \quad |z| > \dfrac{L}{2} \end{matrix} \right. . \tag{12}$$

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

$$\varepsilon_{c1} \left\{ \begin{matrix} th\left(\varepsilon_{b1} \dfrac{qL}{2} \right) \\ cth\left(\varepsilon_{b1} \dfrac{qL}{2} \right) \end{matrix} \right\} - \varepsilon_{c2} = 0 \tag{13}$$

within the frequency region when the inequalities are valid $\varepsilon_{1z}(\omega)\varepsilon_{2z}(\omega) < 0$, $\varepsilon_{1\perp}(\omega)\varepsilon_{1z}(\omega) > 0$ i $\varepsilon_{2\perp}(\omega)\varepsilon_{2z}(\omega) > 0$.

In formulas (12), (13) the following notation is introduced:

$$\varepsilon_{ci}(\omega) = \sqrt{\varepsilon_{i\perp}\varepsilon_{iz}}, \quad \varepsilon_{bi}(\omega) = \sqrt{\varepsilon_{i\perp} \big/ \varepsilon_{iz}}, \quad i = 1, 2, \dots .$$

For the confined phonons (symmetric and antisymmetric) $V(q)$ is as follows:

$$V_C^{\left\{ \begin{smallmatrix} S \\ A \end{smallmatrix} \right\}}(q) = V_C^{(1)}(\vec{q}) \cdot V_C^{(2)}(\vec{q}, z) =$$

$$= \frac{\dfrac{C}{\sqrt{S}}}{\sqrt{\dfrac{\partial}{\partial \omega} \left(\varepsilon_{1\perp} q^2 + \varepsilon_{1z} k_m^2 \right) \dfrac{L}{2} - 2q \dfrac{\partial}{\partial \omega} \left\{ \begin{matrix} f_S(\omega) \cos\left(\dfrac{k_m L}{2} \right) \\ f_A(\omega) \sin\left(\dfrac{k_m L}{2} \right) \end{matrix} \right\}}} \times$$

$$\times \left\{ \begin{matrix} \left\{ \begin{matrix} \cos(k_m z) \\ \sin(k_m z) \end{matrix} \right\}, \quad |z| < \dfrac{L}{2} \\ \left\{ \begin{matrix} \cos\left(\dfrac{k_m L}{2} \right) \\ \operatorname{sgn}(z) \sin\left(\dfrac{k_m L}{2} \right) \end{matrix} \right\} \exp\left[-\kappa_2 \left(|z| - \dfrac{L}{2} \right) \right], |z| > \dfrac{L}{2}, \end{matrix} \right. \tag{14}$$

where

$$\left\{ \begin{matrix} f_S(\omega) \\ f_A(\omega) \end{matrix} \right\} = \operatorname{sgn}(\varepsilon_{1z}) \sqrt{-\varepsilon_{1\perp}(\omega)\varepsilon_{1z}(\omega)} \times$$

$$\times \left\{ \begin{matrix} \sin\left(\dfrac{k_m L}{2} \right) \\ \cos\left(\dfrac{k_m L}{2} \right) \end{matrix} \right\} - \operatorname{sgn}(\varepsilon_{2z}) \varepsilon_{c2} \left\{ \begin{matrix} \cos\left(\dfrac{k_m L}{2} \right) \\ \sin\left(\dfrac{k_m L}{2} \right) \end{matrix} \right\},$$

k_m is determined from

$$\varepsilon_{1z} k_m \left\{ \begin{matrix} \sin\left(\dfrac{k_m L}{2} \right) \\ \cos\left(\dfrac{k_m L}{2} \right) \end{matrix} \right\} - \varepsilon_{2z} \kappa_2 \left\{ \begin{matrix} \cos\left(\dfrac{k_m L}{2} \right) \\ \sin\left(\dfrac{k_m L}{2} \right) \end{matrix} \right\} = 0,$$

under the condition that $\dfrac{\pi}{L} \left\{ \begin{matrix} 2m \\ 2m-1 \end{matrix} \right\} < k_m < \dfrac{\pi}{L} \left\{ \begin{matrix} 2m+2 \\ 2m+1 \end{matrix} \right\}$.

For the symmetric and antisymmetric phonons m = 0,1,2,… and m=1,2,3,…, respectively.

The semiconfined polarization phonons – their $E_\perp$ and D_z 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 $V(\mathrm{Q})$ for the symmetric, antisymmetric phonon modes:

$$V_{HS}^{\left\{ \begin{smallmatrix} S \\ A \end{smallmatrix} \right\}}(\vec{Q}) = V_{HS}^{(1)}(\vec{Q}) V_{HS}^{(1)}(\vec{Q}, z) =$$

$$= \frac{C}{\sqrt{\tilde{L} S}} \left[\frac{\partial}{\partial \omega} \left(\varepsilon_{2\perp} \sin^2 \theta_2 + \varepsilon_{2z} \cos^2 \theta_2 \right) \right]^{-1/2} \frac{\sqrt{2}}{Q} \times \tag{15}$$

$$\times \left[\varepsilon_{1z}^2 \kappa_1^2 \left\{ \begin{matrix} sh^2\left(\dfrac{\kappa_1 L}{2} \right) \\ ch^2\left(\dfrac{\kappa_1 L}{2} \right) \end{matrix} \right\} + \varepsilon_{2z}^2 Q_z^2 \left\{ \begin{matrix} ch^2\left(\dfrac{\kappa_1 L}{2} \right) \\ sh^2\left(\dfrac{\kappa_1 L}{2} \right) \end{matrix} \right\} \right]^{-1/2} \times$$

$$\times\begin{cases}\left\{\begin{Bmatrix}1\\ \operatorname{sgn}(z)\end{Bmatrix}\varepsilon_{1z}\kappa_1\begin{Bmatrix}\dfrac{sh\left(\frac{\kappa_1 L}{2}\right)}{ch\left(\frac{\kappa_1 L}{2}\right)}\end{Bmatrix}\sin\left(Q_z\left(|z|-\frac{L}{2}\right)\right)+\right.\\ \left.+\varepsilon_{2z}Q_z\begin{Bmatrix}\dfrac{ch\left(\frac{\kappa_1 L}{2}\right)}{sh\left(\frac{\kappa_1 L}{2}\right)}\end{Bmatrix}\cos\left(Q_z\left(|z|-\frac{L}{2}\right)\right)\right\}, |z|>\dfrac{L}{2}\\ \varepsilon_{2z}Q_z\begin{Bmatrix}ch(\kappa_1 z)\\ sh(\kappa_1 z)\end{Bmatrix}, \quad |z|<\dfrac{L}{2}\end{cases}$$

where the angle θ_2 is the one between the phonon wave vector $\vec{\mathrm{Q}}=\left(\vec{q},\mathrm{Q}_z\right)$ and the z-axis.

Eqs. (15) are valid when the inequality $\varepsilon_{1\perp}\varepsilon_{1z}>0$ is satisfied, because only in this case vibrations will decay in the nanofilm region, since $\kappa_1=\sqrt{\dfrac{\varepsilon_{1\perp}(\omega)}{\varepsilon_{1z}(\omega)}}q$.

Another type of vibrations – the ones that spread in the medium – can exist only when the two inequalities are fulfilled

$$\varepsilon_{1\perp}(\omega)\varepsilon_{2z}(\omega)<0, \quad \varepsilon_{2\perp}(\omega)\varepsilon_{2z}(\omega)<0. \tag{16}$$

The analysis shows that there is no frequency region in the AlN/GaN/AlN heterosystem where inequalities (16) are satisfied, therefore the above-mentioned phonons do not exist in the heterosystem under consideration [7].

In order to determine the electron energy, one must solve the Schrödinger equation with Hamiltonian (3)

$$\hat{H}_e\psi_e(\vec{r})=E_e\psi_e(\vec{r}). \tag{17}$$

The electron potential energy in the heterosystem is chosen as a rectangular potential well

$$V(z)=\begin{cases}0, & |z|<\dfrac{L}{2}\\ V_0, & |z|\geq\dfrac{L}{2}\end{cases}. \tag{18}$$

Then the wave function looks as follows:

$$\psi_e(\vec{r})=\frac{1}{\sqrt{S}}e^{i\vec{k}\vec{\rho}}\varphi_n(z),$$

$$\text{where } \varphi_n(z)=\begin{cases}Ae^{\chi_0 z}, & z<-L/2\\ \alpha\sin(\chi z)+\beta\cos(\chi z), & |z|<L/2\\ Be^{-\chi_0 z}, & z>L/2\end{cases},$$

$$\chi_0=\sqrt{\frac{2m_{\|2}}{\hbar^2}\left(V_0-E\right)},\ \chi=\sqrt{\frac{2m_{\|1}}{\hbar^2}E},$$

and the electron energy is described by

$$E_n\left(\vec{k}\right)=\frac{p^2}{2m_\perp}+\tilde{E}_n, \tag{19}$$

$\vec{p}$ is the electron impulse, and $\tilde{E}_n$ is found from the dispersion relation by applying the boundary conditions for both the wave function and its probability current density at the interface.

In order to determine the polaron energy, the perturbation theory and the variational Lee-Low-Pines (LLP) method are used [17, 18]. 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 (2) is averaged over the functions of the electron ground stationary state in the motion along the z-axis

$$\hat{H}_{ef}=\left\langle\varphi_1(z)\middle|\hat{H}\middle|\varphi_1(z)\right\rangle=$$

$$=\tilde{E}_1+\frac{p^2}{2m_\perp}+\hat{H}_{ph}+\sum_{\vec{q}}V^{(1)}(\vec{q})\left(e^{i\vec{q}\vec{\rho}}M_{11}b_{\vec{q}}+e.c.\right), \tag{20}$$

where $M_{1n}=\int\limits_{-\infty}^{\infty}\varphi_1^*(z)V^{(2)}(\vec{q},z)\varphi_n(z)dz$, $n=1$.

To Hamiltonian (20), two unitary transformations are consecutively applied by operators

$$\hat{S}=\exp\left[\frac{i}{\hbar}\left(\vec{P}-\sum_{\vec{q}}b_{\vec{q}}^{+}b_{\vec{q}}\hbar\vec{q}\right)\vec{\rho}\right],$$

$$\hat{U}=\exp\left[\sum_{\vec{q}}\left(b_{\vec{q}}^{+}f(\vec{q})-b_{\vec{q}}f^*(\vec{q})\right)\right],$$

where $\vec{P}=\hbar\vec{k}$ is the polaron impulse.

After averaging of the obtained expression over the vacuum phonon state and minimizing of the functional over $f(\vec{q})$ and $f^*(\vec{q})$, the polaron energy of the heterosystem is found [20-22]

$$E_{pol}\left(\vec{k}\right)=\tilde{E}_1+\frac{\hbar^2k^2}{2m_\perp}\left(1+\eta^2\right)+$$

$$+\sum_{\vec{q}}\frac{-2\cdot\left|V^{(1)}(\vec{q})\right|^2\left|M_{11}\right|^2}{\hbar\omega-\frac{\hbar\vec{q}\vec{P}}{m_\perp}(1-\eta)+\frac{\hbar^2q^2}{2m_\|}}+$$

$$+\sum_{\vec{q}}\frac{\left|V^{(1)}(\vec{q})\right|^2\left|M_{11}\right|^2\left\{\hbar\omega-\frac{\hbar\vec{q}\vec{P}}{m_\perp}+\frac{\hbar^2q^2}{2m_\perp}\right\}}{\left\{\hbar\omega-\frac{\hbar\vec{q}\vec{P}}{m_\perp}(1-\eta)+\frac{\hbar^2q^2}{2m_\perp}\right\}^2}, \tag{21}$$

where $\eta\vec{P} = \sum_{\vec{q}} \left| f_{\min}\left(\vec{q}\right) \right|^2 \hbar\vec{q}$,

$$f_{\min}\left(\vec{q}\right) = -\frac{V^{(1)*}\left(\vec{q}\right) M_{11}^{*}}{\hbar\omega + \frac{\hbar^2 q^2}{2m_\perp} - \frac{\hbar^2}{m_\perp}\vec{k}\vec{q}\left(1-\eta\right)}.$$

The polaron energy in the bulk material is determined by similar formulas [17]. The difference is that expression (21) contains the function M_{11}, resulting from the translational symmetry deviation of the system in the z-direction.

The crystals AlN, GaN are characterized by the small constant of the electron-phonon interaction ($\alpha = 0.681$, $\alpha = 0.466$ respectively), therefore to determine the polaron energy, one can use perturbation theory [14, 15]

$$E_{pol}\left(\vec{k}\right) = \tilde{E}_1 + \frac{\hbar^2 k^2}{2m_\perp} + \sum_{n,\vec{q}} \frac{\left|V^{(1)}\left(\vec{q}\right)\right|^2 \left|M_{1n}\right|^2}{\tilde{E}_1 - \tilde{E}_n - \hbar\omega + \frac{\hbar^2 k^2}{2m_\perp} - \frac{\hbar^2\left(\vec{k}-\vec{q}\right)^2}{2m_\perp}}. \quad (22)$$

In receiving of formula (22), the adiabatic approach was not used, thus it can be applied nod only for the small values L of quantum well widths. Expressions (21) and (22) reflect the wave-vector dependence of the polaron energy, i.e. the quasiparticle dispersion relation.

3. Results and discussion

In the study of polaron states, we consider a small range of the wave-vector change ($k \approx 0$). The quantities $\eta\left(\vec{k}\right)$ and $E_{pol}\left(\vec{k}\right)$ are obtained by expanding of the corresponding expressions in series and taking only their first terms [17]. Regarding the polaron dispersion relation in a small but finite region of the wave-vector change $0 \le k < k_f$, $k_f = \sqrt{\frac{2m_\perp\hbar\omega}{\hbar}} << k_0$ (where k_0 is the wave-vector critical value in the Brillouin zone), the calculations $E_{pol} = E_{pol}\left(\vec{k}\right)$ were carried out without any additional simplification of formulas (21), (22). Material parameters are taken to be $\varepsilon^{\infty} = 5.29$, $\omega_{\perp L} = 743\,cm^{-1}$, $\omega_{zL} = 735\,cm^{-1}$, $\omega_{\perp} = 561\,cm^{-1}$, $\omega_z = 533\,cm^{-1}$ for GaN. For AlN, we use $\varepsilon^{\infty} = 4.68$, $\omega_{\perp L} = 916\,cm^{-1}$, $\omega_{zL} = 893\,cm^{-1}$, $\omega_{\perp} = 673\,cm^{-1}$, $\omega_z = 660\,cm^{-1}$ [6].

It is seen from the above-defined formulas that the functions of the electron interaction with different polarization oscillation phonon modes of the hexagonal symmetry crystal heterostructure are complex. Therefore, it is worth examining the functions which assist to calculate electron dispersion probabilities on these phonons. For non-dimensional wave vectors ($q = \tilde{q}\frac{\pi}{a}$), this function is as follows:

$$\Phi\left(\tilde{q}\right) = \frac{\pi S}{2a^2}\left|V^{(1)}\right|^2 \left|M_{1n}\right|^2 \tilde{q},$$

where a is the lattice constant.

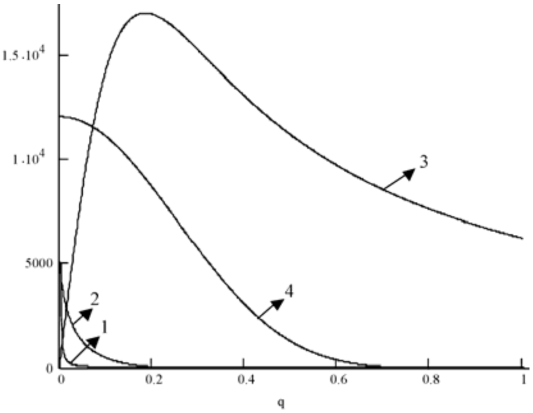


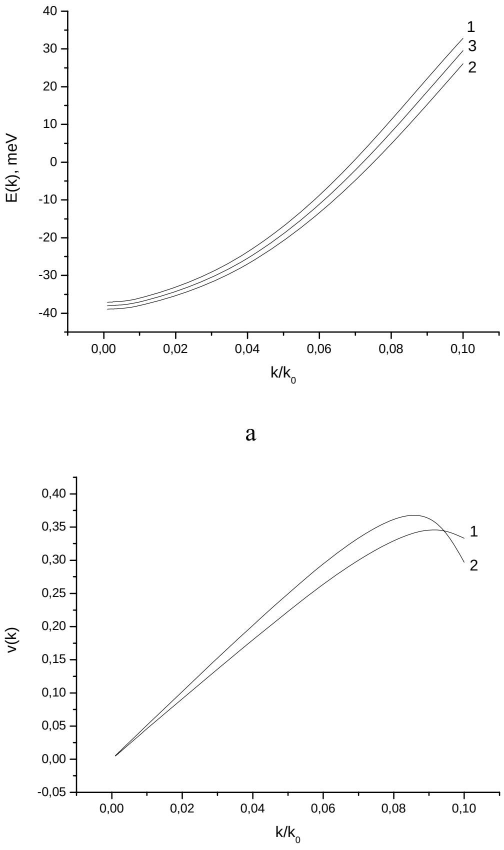
Fig.1. Dependence of the function Φ=Φ(q) for half-space (1), interface (2), confined (3) polarization phonons and bulk crystal phonons (4) at L=25 Å and n=1.

Fig.1 shows the dependence of this function in the particular case of the AlN/GaN/AlN heterosystem for three types of polarization phonons (confined, interface, half-space) at L = 25 Å and $n = 1$. Similar dependences are received at L = 50, 75, 100, 125, 150 Å. The analysis shows that for small nanofilm thickness values the interface phonons make a significant contribution in the polaron energy. The rise of L leads to the reduction of this contribution. If L > 100 Å, then in the polaron energy formation it is confined phonons that play a dominant role.

Note one more result. In Fig.1, curve 4 in the integral form reflects the behaviour of curves 1-3. Thus, if one chooses the model for heterosystem polarization phonons to remain analogous to that of the bulk crystal, the energy calculation results will be in a good agreement with the data derived for all types of polarization oscillations [20-22]. This property of polarization phonons is rather general. It can be proved that the form-factor assigned to the effective interelectron interaction due to polarization vibrations for bulk crystal phonons is equal to the sum of all polarization-mode form-factors of the heterosystem [18].

For the sake of simplicity, the zero level of the polaron energies is set at the electron first level energy

$\tilde{E}_1$. In this case it is possible to compare the polaron energies in different quantum wells as well as in a bulk crystal.



a

b

Fig. 2. (a) Polaron dispersion relation for the GaN crystal in the cases of $\theta = 0$ *(1),* $\theta = \pi/2$ *(2),* $\theta = \pi/4$ *(3). (b) Polaron average speed for the GaN crystal in the cases of* $\theta = 0$ *(1),* $\theta = \pi/2$ *(2).*

Fig.2*a* demonstrates the calculation results of the polaron dispersion relation in the range $k < k_f$ for the GaN crystal in different polaron wave-vector directions with respect to the *C*-axis of the crystal (angles θ_k). As is seen, the function $E_{pol} = E_{pol}(\vec{k})$ depends not only on the wave-vector module but also on the angle θ_k at all values of k. Besides in the range of very small k, the dispersion relation has parabolic character. The increase of k is followed by "deformations" of the dispersion relation. The latter result is well seen from the dependence of the polaron average speed

$$\upsilon = \frac{1}{\hbar}\left|\nabla E_{pol}(\vec{k})\right| \tag{24}$$

In the small k values region, the average speed is a linear function of k (Fig.2*b*). The difference between the curves is determined by the initial electron mass which varies in different directions. However, the further rise of k results in the deviation of $\upsilon = \upsilon(\vec{k})$ from a linear dependence. Obviously, such behaviour of $\upsilon = \upsilon(\vec{k})$ should influence the electric and optoelectric crystal properties.

The above-mentioned properties of $E_{pol} = E_{pol}(\vec{k})$ and $\upsilon = \upsilon\left(\vec{k}\right)$ are also typical of the AlN*/GaN/AlN* double heterosystem. In this case the calculations show the enhancement of all characteristics of the dispersion relation and speed. Fig.3 illustrates that the polaron binding energy ($E_C \equiv \left|E_{pol}(0)\right|$) in the GaN bulk crystal is smaller than that in the heterosystem. The reduction of quantum well width (*L*) leads to the increase of this energy and the dispersion relation deformation growth.

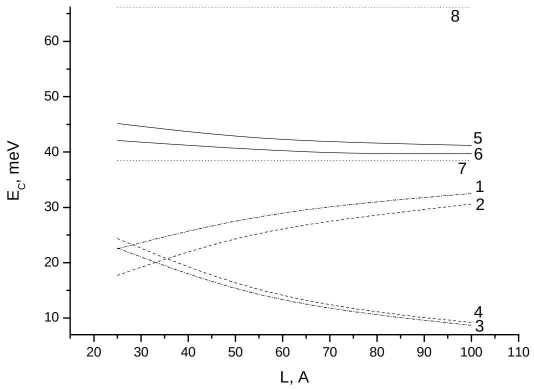


Fig.3 Polaron binding energy of the GaN (7) and AlN (8) bulk crystals, and AlN/GaN/AlN heterosystem in the case of IQW (curves 1,3,5), FQW (curves 2,4,6). 1,2 stand for confined phonons, 3,4 regard for interface phonons, 5,6 stand for all phonons.

As to partial contributions, the confined phonons are predominant at *L* > 40 Å, though one cannot neglect interface phonon contributions in the range of 40 Å < *L* < 100 Å. For thicknesses of *L* < 30 Å the interface phonon contribution becomes greater than that of the confined phonons. As to the half-space phonon contribution, the calculations show that they have little effect on the polaron binding energy. For illustration, at *L* = 25 Å for the AlN/GaN/AlN double heterostructure within the infinite quantum well (IQW) model, the contribution makes in the case of confined phonons 22.536 meV, interface phonons

22.633 meV, and half-space phonons 2.035 meV, while at L = 100 Å it is 32.484 meV, 8.711 meV, 1.184 meV respectively. Comparison of two models – the IQW ($V = \infty$ in formula (18)) 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 $L < 60$ Å (e.g. if L = 50 Å, it makes 17%)).

Fig.4 shows the dependence of the dispersion relation of a polaron that moves parallel to the heterosystem interfaces at L < 25 Å. In the range of wave-vector small 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 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 $V_0 = \infty$ model is smaller than that for the finite value of V_0. However, the wave-vector growth is followed by the reduction of the polaron energy difference within different QW models.

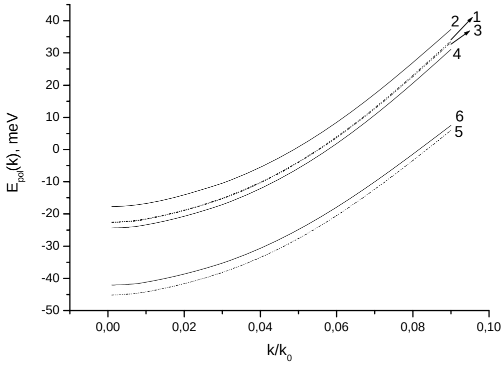


Fig. 4. Polaron energy of the heterosystem AlN/GaN/AlN for QW at L = 25 Å in the case of IQW (curves 1,3,5), FQW (curves 2,4,6). 1,2 show the energy with regard for confined phonons, 3,4 stand for the interface phonons, 5,6 stand for all phonons.

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

$$\vec{v} = \frac{1}{\hbar}\nabla_{\vec{k}} E_{pol}(\vec{k}) \tag{25}$$

This quantity enters the formulas of kinetic coefficients as well as defines the degree of polaron dispersion relation "deformation". It is seen from Fig.5 that in the region of small wave-vector values, the increase of k – as a result of all phonon modes contribution – results in $v = v(k)$ approaching saturation, i.e., the polaron dispersion relation $E_{pol} = E_{pol}(k)$ transfers from a quadratic function (at $k = 0$) into a liner one (at $k = k_f$).

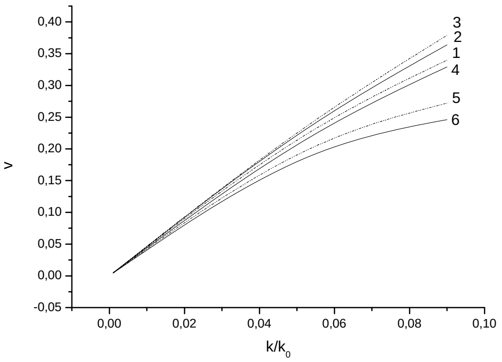


Fig.5. Polaron average speed of the AlN/GaN/AlN heterosystem for QW with L = 25Å in the cases of IQW (curves 1,3,5) and FQW (curves 2,4,6). 1,2 regard for the interaction with confined phonons, 3,4 take account of interface phonons, 5,6 regard for all phonons.

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

$$\frac{1}{m_p} = \frac{1}{\hbar^2}\left.\frac{\partial^2 E_{pol}(k)}{\partial k^2}\right|_{k=0} \tag{26}$$

Fig.6 depicts 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.

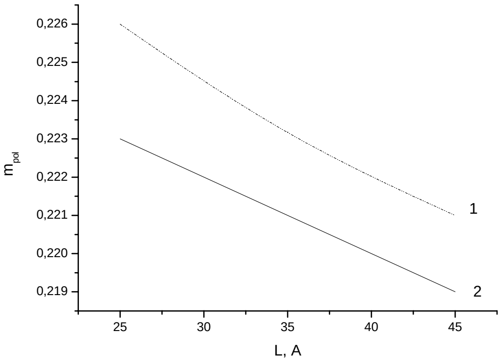


Fig. 6. Polaron effective mass of the AlN/GaN/AlN heterosystem in the case of IQW (1), FQW (2) with regard for all phonons.

4. Conclusions

Therefore, the report presents a theoretical study of the polaron dispersion relation in the GaN crystal and 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 band gaps. Calculations of the average speed and the polaron effective mass are performed. It is shown that when a nanofilm thickness increases, the interface phonon contribution in the polaron energy decreases, while that of the confined phonons grows. The calculation results of the polaron dispersion relation in the region of $k < k_f$ 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 and increase of the wave-vector k cause an effective enhancement of the electron-phonon interaction.

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[*] Corresponding author: vika.borusevych@gmail.com