doi: 10.15407/ujpe62.11.0984

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POLARON STATE IN THE SELF-CONSISTENT ELECTRON-DEFORMATION FIELD OF THE "QUANTUM DOT-MATRIX" SYSTEM

PACS 71.38.-k, 73.63.Kv

The potential well depth for an electron in a nanoheterosystem with quantum dots has been calculated in the framework of the self-consistent electron-deformation model. It is shown that the strained InAs/GaAs nanoheterosystem with InAs spherical quantum dots is characterized by deformation fields, which appear at the quantum dot-matrix interface and result in the enhancement of polaron effects in comparison with the unstrained material. The electron polaron energy is calculated, by considering the electrostatic energy and the energy associated with the mechanical and electron-deformation strain components in the quantum-dot and matrix materials.

K e y w o r d s: quantum dot, polaron, electron-deformation potential, binding energy, electron.

1. Introduction

Nowadays, a large attention is focused on the researches dealing with quantum-size structures, in particular, quantum dots (QDs), which find the wide application in nanoelectronics as field-effect transistors, photo cells, light-emitting diodes, and lasers [1, 2]. In low-dimensional systems, the electron-phonon interaction can significantly affect the physical properties of electrons, such as the electron scattering, polaron effects, and so forth [3, 4]. A deformation that arises at the QD-matrix interface owing to the mismatch of lattice parameters results in the emergence of the deformation and piezoelectric fields, which affect the optical properties of those objects. In particular, the compressive deformation of a QD material in the matrix (e.g., InAs in GaAs and CdTe in ZnTe) enhances the localization of charged quasiparticles and excitons in those QDs and considerably strengthens the interaction of quasiparticles both with one another and with longitudinal optical phonons. Furthermore, the materials of those QDs are characterized by a high deformation potential, which results in the enhancement of polaron effects in comparison with bulk materials.

Various approaches are used to study polaron effects in nanostructured materials: Feynman's method of path integration, the method of canonical transformations [5, 6], and the Buimistrov–Pekar method [7]. In particular, in work [8], the binding energy of electron and hole polarons in spherical QDs with an infinitely deep potential well created on the basis of materials with a high ionicity was calculated, by neglecting a lattice deformation in the QD material. The influence of a deformation emerging only due to a mismatch between the QD and matrix lattice parameters on polaron effects was studied in work [9].

In this work, the binding energy of an electron polaron is calculated with regard for the electron-deformation and electrostatic potentials in an InAs/GaAs nanoheterosystem with strained spherical InAs quantum dots.

2. Geometric Model of a Strained Nanoheterosystem with Quantum Dots

Let us consider an InAs/GaAs nanoheterosystem with strained InAs quantum dots. The latter do not have a pronounced crystallographic faceting. In particular, the QD shape is approximately spherical. For example, QDs of this geometry are formed in the InAs/GaAs(001) nanoheterosystem, when the thickness of the growing InAs layer is about 2 monolayers [10]. Therefore, in what follows, the contribution of island edges to the elastic relaxation energy is neglected.

An ordered arrangement of strained QDs in a crystalline matrix takes place owing to the elastic in-

teraction between the islands. This interaction arises as a result of the parameter mismatch between the InAs/GaAs lattices. In order to reduce the problem with a large number of QDs to a problem with a single QD, the following approximation was made. The energy of the elastic interaction between two QDs was substituted by the interaction energy of both those QDs with the averaged field of elastic deformations created by all other QDs, $\sigma_{\rm ef}(N-1)$. In InAs/GaAs quantum dots grown in the Stranski–Krastanov mode, the strong deformation fields appear at the QD-matrix interface because of the InAs/GaAs lattice parameter misnatch, $f = (a^{(1)} - a^{(2)})/a^{(2)} \approx \approx 7\%$ [11].

As was shown in works [8, 9], the polaron effects grow with a reduction of the QD size. The enhancement parameter p is equal to the ratio between the radii of the polaron state, a_0, and a quantum dot, R_0, i.e. $p = a_0/R_0 \gg 1$. In the case where the QD material is subjected to a compressive deformation, the enhancement parameter p grows, because the QD size R_0 decreases: firstly, owing to the mechanical compressive deformation in the QD material that arises as a result of the parameter mismatch between the contacting (QD and matrix) lattices and, secondly, owing to the electron-deformation component

$$\mathrm{Sp}\,\hat{\varepsilon} = \mathrm{Sp}\,\hat{\varepsilon}^{(1)}_{\rm mech}(r) + \mathrm{Sp}\,\hat{\varepsilon}^{(1)}_{\rm el-def}(r)) < 0,$$

where $\mathrm{Sp}\,\hat{\varepsilon}^{(1)}_{\rm (mech)}$ is the sum of the diagonal components in the mechanical strain tensor for the QD material, and $\mathrm{Sp}\,\hat{\varepsilon}^{(1)}_{\rm el-def}(r)$ is the sum of the diagonal components in the tensor of electron-deformation strain component [12]. Self-consistent electron-deformation effects, which arise due to the coupling between the lattice deformation and the electron subsystem, additionally enhance polaron effects in comparison with those governing by the mechanical deformation only:

$$p = \frac{a_0}{R_0\,(1 - |\mathrm{Sp}\,\hat{\varepsilon}|)}. \tag{1}$$

The strain tensor components are determined from the balance equation. In the case of spherical symmetry, this equation looks like

$$\frac{d^2u_r^{(i)}}{dr^2} + \frac{2}{r}\frac{du_r^{(i)}}{dr} - \frac{2}{r^2}u_r^{(i)} = D^{(i)}e\frac{d\phi^{(i)}(r)}{dr}, \tag{2}$$

where $\mathbf{u}(\mathbf{r})$ is the atomic displacement in the QD material, which should satisfy the following boundary conditions [13–15]:

$$\begin{cases} 4\pi R_0^2\left(u_r^{(2)}\big|_{r=R_0} - u_r^{(1)}\big|_{r=R_0}\right) = \Delta V, \\ \sigma_{rr}^{(1)}\big|_{r=R_0} = \sigma_{rr}^{(2)}\big|_{r=R_0} - P_{\rm L}, \quad P_{\rm L} = \dfrac{2\alpha}{R_0}, \\ \sigma_{rr}^{(2)}\big|_{r=R_1} = -\sigma_{\rm ef}\,(N-1), \end{cases} \tag{3}$$

R_0 is the radius of a nondeformed QD, R_1 the matrix radius, $P_{\rm L}$ the Laplace pressure,

$$\Delta V = f4\pi R_0^3, \quad \alpha = \frac{2\int_0^{R1}\rho^{(i)}(c^{(i)})^2(\varepsilon^{(i)})^2(r)r^2dr}{R_0u_r^{(1)}(R_0)}$$

is the interphase free energy between the QD and matrix materials [16], $c^{(i)}$ the longitudinal acoustic velocity in the i-th medium ($i = 1$ for InAs and 2 for GaAs), $\rho^{(i)}$ the density of the i-th medium, and

$$D^{(i)} = \frac{(1+\nu^{(i)})(1-2\nu^{(i)})}{(a^{(i)})^3E^{(i)}(1-\nu^{(i)})}.$$

The mechanical strains in the QD, $\sigma_{rr}^{(1)}$, and matrix, $\sigma_{rr}^{(2)}$, materials equal

$$\sigma_{rr}^{(i)} = \frac{E_i}{(1+\nu_i)\,(1-2\nu_i)}\Big[(1-\nu_i)\,\varepsilon_{rr}^{(i)} + \\ + \nu_i\left(\varepsilon_{\varphi\varphi}^{(i)} + \varepsilon_{\theta\theta}^{(i)}\right)\Big], \tag{4}$$

where ν_i and E_i are Poisson's ratio and the Young modulus, respectively, for the i-th material.

The general solution of the inhomogeneous equation (2) is the sum of the mechanical and electron-deformation displacement components,

$$u_r^{(i)}(r) = u_{\rm rmech}^{(i)}(r) + u_{\rm rel-def}^{(i)}(r), \tag{5}$$

where

$$u_{r\rm mech}^{(i)}(r) = C_1^{(i)}r + \frac{C_2^{(i)}}{r^2}, \tag{6}$$

$$u_{\rm rel-def}^{(i)}(r) = \frac{D^{(i)}e}{r^2}\int r'^2\phi^{(i)}(r')dr'. \tag{7}$$

The displacement must be finite at $r = 0$. Therefore, we must put

$$C_2^{(1)} = 0 \tag{8}$$

in solution (6). The displacement field determines the strain tensor components for the QD material,

$$\varepsilon^{(1)}_{rr\text{mech}} = \varepsilon^{(1)}_{\varphi\varphi\text{mech}} = \varepsilon^{(1)}_{\theta\theta\text{mech}} = C^{(1)}_1, \tag{9}$$

and the material of the surrounding matrix,

$$\begin{aligned} &\varepsilon^{(2)}_{rr\text{mech}} = C^{(2)}_1 - \frac{2C^{(2)}_2}{r^3}, \\ &\varepsilon^{(2)}_{\varphi\varphi\text{mech}} = \varepsilon^{(2)}_{\theta\theta\text{mech}} = C^{(2)}_1 + \frac{C^{(2)}_2}{r^3}. \end{aligned} \tag{10}$$

The mechanical component of a uniform strain equals

$$\varepsilon^{(i)}_{\text{mech}} = \varepsilon^{(i)}_{rr\text{mech}} + \varepsilon^{(i)}_{\varphi\varphi\text{mech}} + \varepsilon^{(i)}_{\theta\theta\text{mech}} = 3C^{(i)}_1. \tag{11}$$

Therefore, $\text{Sp}\,\hat{\varepsilon}^{(1)}_{(\text{mech})} = 3C^{(1)}_1$.

The field of electron-deformation displacements is described by the following components of the electron-deformation tensor:

$$\varepsilon^{(i)}_{rr\text{el}-\text{def}} = D^{(i)} e \left(\frac{2}{r^3} \int r'^2 \phi^{(i)}(r') dr' - \phi^{(i)}(r') \right), \tag{12}$$

$$\varepsilon^{(i)}_{\varphi\varphi\text{el}-\text{def}} = \varepsilon^{(i)}_{\theta\theta} = D^{(i)} e \left(\frac{1}{r^3} \int r'^2 \phi^{(i)}(r') dr' \right). \tag{13}$$

The electron-deformation component of a uniform strain equals

$$\varepsilon^{(i)}_{\text{el}-\text{def}} = \varepsilon^{(i)}_{rr\text{el}-\text{def}} + \varepsilon^{(i)}_{\varphi\varphi\text{el}-\text{def}} + \varepsilon^{(i)}_{\theta\theta\text{el}-\text{def}} = D^{(i)} e \varphi^{(i)}(r). \tag{14}$$

Therefore,

$$\text{Sp}\,\varepsilon^{(1)}_{\text{el}-\text{def}}(r) = D^{(1)} e \varphi^{(1)}(r). \tag{15}$$

The potential $\varphi^{(i)}(\mathbf{r})$ is determined from the Poisson equation

$$\Delta\varphi^{(i)}(\mathbf{r}) = \frac{e}{\varepsilon^{(i)}_d \varepsilon_0} \Delta n^{(i)}(\mathbf{r}), \tag{16}$$

where $\varepsilon^{(i)}_d$ is the relative dielectric permittivity of the i-th material in the nanoheterosystem, and $\Delta n^{(i)}(\mathbf{r}) = n^{(i)}(\mathbf{r}) - n_0$ is a change of the electron concentration in a vicinity of the hetero-interface "QD-matrix". The electron concentration itself is determined in terms of the superposition of wave-function products,

$$n^{(i)}(\mathbf{r}) = \sum_n \frac{\psi^{*(i)}_n(\mathbf{r}) \psi^{(i)}_n(\mathbf{r})}{\exp\left(\frac{E_n - \mu}{kT}\right) + 1}, \tag{17}$$

In turn, the wave functions are found from the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m^{*(i)}} \Delta_{\mathbf{r}} + \Delta V_c(\mathbf{r}) \right] \psi^{(\text{i})}_{\text{n0}}(\mathbf{r}) = E_n \psi^{(\text{i})}_{\text{n0}}(\mathbf{r}) \tag{18}$$

with the boundary conditions

$$\begin{cases} R^{(1)}_{nl}(r)\big|_{r=R_0} = R^{(2)}_{nl}(r)\big|_{r=R_0}; \\ \dfrac{1}{m^{*(1)}} \dfrac{dR^{1)}_{nl}(r)}{dr}\Big|_{r=R_0} = \dfrac{1}{m^{*(2)}} \dfrac{dR^{(2)}_{nl}(r)}{dr}\Big|_{r=R_0}, \end{cases} \tag{19}$$

where $m^{*(i)}$ is the effective electron mass in the i-th material, E_n the energy of an electron on the n-th level in the quantum well,

$$\Delta V_c(r) = \left(\Delta E_c(0) + a^{(2)}_c \left(\varepsilon^{(2)}_{\text{mech}}(r) + \varepsilon^{(2)}_{\text{el}-\text{def}}(r) \right) - a^{(1)}_c \left(\varepsilon^{(1)}_{\text{mech}}(r) + \varepsilon^{(1)}_{\text{el}-\text{def}}(r) \right) - e \left(\phi^{(2)}(r) - \phi^{(1)}(r) \right) \right)$$

is the potential energy of an electron in the QD, $\Delta E_c(0)$ the potential well depth for an electron in the unstrained QD, $a^{(i)}_c$ the constant of the hydrostatic deformation potential of the conduction band, n_0 the average concentration of conduction electrons, $n^{(i)}(\mathbf{r})$ the concentration of charge carriers in the i-th material of the strained nanoheterostructure with the QD, and μ the chemical potential of the nanoheterostructure. The latter quantity is determined by the equation

$$\frac{1}{\Omega_0} \int n(\mathbf{r}) d\mathbf{r} = n_0, \tag{20}$$

where Ω_0 is the unit cell volume.

The required solution of the Schrödinger equation (18) written in the spherical coordinate system is sought in the form

$$\psi^{(i)}_{nlm}(r, \theta, \varphi = R^{(i)}_{nl}(r)\, Y^{(i)}_{lm}(\theta, \varphi),$$

where $Y^{(i)}_{lm}(\theta, \varphi)$ are the spherical functions. With regard for the relation $\overline{\Delta\varphi(r, \theta, \varphi)} = \Delta_r \varphi(r)$ [22], the Poisson equation (16) in the spherical symmetry case looks like

$$\frac{d^2\varphi^{(i)}}{dr^2} + \frac{2}{r} \frac{d\varphi^{(i)}}{dr} = \frac{e}{\varepsilon^{(i)}_d \varepsilon_0} n^{(i)}(r) - n_0, \tag{21}$$

where $\varphi(r)$ is the solution averaged over a sphere with the radius r. The concentration of charge carriers in the strained nanoheterostructure with a QD was found to equal [12]

$$n^{(i)}(r) \approx \left| \psi^{(i)}_{nlm} \right|^2 \frac{N_{\text{QD}}}{a_i} \left[\text{erf}\left(\frac{\sqrt{2}}{\Delta E} E_1 \right) \right] +$$

$$+\operatorname{erf}\left(\frac{\sqrt{2}}{\Delta E}\left(\mu-E_1-\lambda_0^{(i)}-a_c^{(i)}\varepsilon_{rr}^{(i)}\right)\right)+$$
$$+\sqrt{\frac{8}{\pi}}\frac{e}{\Delta E}\exp\left(\frac{-2\left(\mu-E_1-\lambda_0^{(i)}-a_c^{(i)}\varepsilon_{rr}^{(i)}\right)^2}{\Delta E^2}\right)\times$$
$$\times\varphi^{(i)}(r), \quad (22)$$

where $N_{\rm QD}$ is the surface concentration of QDs, ΔE the Gaussian half-width, and E_1 the energy of an electron on the first localized level in the quantum well.

The solutions of the Poisson equation (21) in the QD and the matrix, in which expression (22) for the electron concentration was taken into account, were sought for the averaged probability density $\left|\bar{\psi}^{(i)}\right|^2$. As a result, we obtained

$$\varphi^{(1)}(r)=A_1\frac{\sinh\left(\sqrt{\frac{1}{a1}}\right)}{r}-a1\,b1, \quad 0\le r\le R_0, \quad (23)$$

$$\varphi^{(2)}(r)=B_1\frac{\exp\left(-\sqrt{\frac{1}{a2}}r\right)}{r}+B_2\frac{\exp\left(\sqrt{\frac{1}{a2}}r\right)}{r}-$$
$$-a2\,b2-\frac{d2}{2r}\left[\exp\left(-\sqrt{\frac{1}{a2}}r\right)E_i\left(\sqrt{\frac{1}{a2}}r\right)+\right.$$
$$\left.+\exp\left(\sqrt{\frac{1}{a2}}r\right)E_i\left(-\sqrt{\frac{1}{a2}}r\right)\right], \quad R_0\le r\le R_1, \quad (24)$$

where

$$E_i(z)=\int\limits_{-z}^{\infty}\frac{\exp(-t)}{t}dt,$$
$$\frac{1}{a1}=\frac{e^2}{\varepsilon_d^{(1)}\varepsilon_0 a^{(1)}}\left|\bar{\psi}^{(1)}\right|^2 N_{\rm QD}\frac{\sqrt{\frac{8}{\pi}}}{\Delta E}\times$$
$$\times\exp\left(\frac{-2\left(\mu-E_1-\lambda_0^{(1)}-a_c^{(1)}C_1^{(1)}\right)^2}{\Delta E^2}\right),$$
$$\frac{1}{a2}=\frac{e^2}{\varepsilon_d^{(2)}\varepsilon_0 a^{(2)}}\left|\bar{\psi}_{(2)}\right|^2 N_{\rm QD}\frac{\sqrt{\frac{8}{\pi}}}{\Delta E}\times$$
$$\times\exp\left(\frac{-2\left(\mu-E_1-\lambda_0^{(2)}-a_c^{(2)}C_1^{(2)}\right)^2}{\Delta E^2}\right),$$
$$d2=\frac{2a_c^{(2)}C_2^{(2)}e}{\varepsilon_d^{(2)}\varepsilon_0 a^{(2)}}\left|\bar{\psi}^{(2)}\right|^2 N_{\rm QD}\frac{\sqrt{\frac{8}{\pi}}}{\Delta E}\times$$
$$\times\exp\left(\frac{-2\left(\mu-E_1-\lambda_0^{(2)}-a_c^{(2)}C_1^{(2)}\right)^2}{\Delta E^2}\right),$$
$$b1=\frac{e}{\varepsilon_d^{(1)}\varepsilon_0 a^{(1)}}\left|\bar{\psi}^{(1)}\right|^2 N_{\rm QD}\left[\operatorname{erf}\left(\frac{\sqrt{2}}{\Delta E}E_1\right)+\right.$$
$$+\operatorname{erf}\left(\frac{\sqrt{2}}{\Delta E}\left(\mu-E_1-\lambda_0^{(1)}-a_c^{(1)}C_1^{(1)}\right)\right)-$$
$$\left.-\frac{a^{(1)}n_0}{\left|\bar{\psi}^{(1)}\right|^2 N_{\rm QD}}\right],$$
$$b2=\frac{e}{\varepsilon_d^{(2)}\varepsilon_0 a^{(2)}}\left|\bar{\psi}^{(2)}\right|^2 N_{\rm QD}\left[\operatorname{erf}\left(\frac{\sqrt{2}}{\Delta E}E_1\right)+\right.$$
$$+\operatorname{erf}\left(\frac{\sqrt{2}}{\Delta E}\left(\mu-E_1-\lambda_0^{(2)}-a_c^{(2)}C_1^{(2)}\right)\right)-$$
$$\left.-\frac{a^{(2)}n_0}{\left|\bar{\psi}^{(2)}\right|^2 N_{\rm QD}}\right].$$

The coefficients A_1, B_1, and B_2 in expressions (23) and (24) are determined from the continuity conditions across the strained heterointerface for the potentials $\varphi^{(1)}(r)$ and $\varphi^{(2)}(r)$, and the normal components of the electric displacement vectors, as well as the electroneutrality condition:

$$\begin{cases}\varphi^{(1)}(r)\big|_{r=R_0}=\varphi^{(2)}(r)\big|_{r=R_0},\\ \varepsilon^{(1)}\dfrac{\varphi^{(1)}(r)}{dr}\Big|_{r=R_0}=\varepsilon^{(2)}\dfrac{\varphi^{(2)}(r)}{dr}\Big|_{r=R_0},\\ \displaystyle\int\limits_0^{R_0}r^2\Delta n^{(1)}(r)dr+\int\limits_{R_0}^{R_1}r^2\Delta n^{(2)}(r)dr=0.\end{cases} \quad (25)$$

3. Electron Polaron Renormalized by the Self-Consistent Electron-Deformation Interaction in a Quantum Dot

The binding energy of an electron-deformation polaron in the deformed QD of the InAs/GaAs heterosystem is determined from the Schrödinger equation that includes the electron-deformation potential of the conduction band, the energy of the electron-phonon interaction, and the own energy of phonons:

$$\left[\hat{H}_e+\Delta V_c+\sum_q\hbar\omega_q a_q^+a_q+e\sqrt{\frac{2\pi\hbar}{V\varepsilon_d^{(i)}\varepsilon_0}}\times\right.$$

$$\times \sum_q \frac{\sqrt{\omega_q}}{q}\left(a_q e^{i\mathbf{qr}} + a_q^+ e^{-i\mathbf{qr}}\right)\Bigg]\psi_{n0}(\mathbf{r}) = \tilde{E}_n \psi_{n0}(\mathbf{r}), \tag{26}$$

where a_q and a_q^+ are the operators of phonon annihilation and creation, respectively.

Since the enhancement parameter $p \gg 1$, let us use the adiabatic approximation, when finding the polaron energy. In this approximation, the electron motion in the QD is fast, whereas the polaron motion is slow. Let us average Eq. (26), by using the wave functions of the zeroth-order approximation, $\psi_{n0}^{(i)}(\mathbf{r})$. The latter are found from the Schrödinger equation

$$\hat{H}_{0e}^{(i)}\psi_{n0}^{(i)}(\mathbf{r}) = E_{n0}\psi_{n0}^{(i)}(\mathbf{r}) \tag{27}$$

with the Hamiltonian

$$\hat{H}_{0e}^{(i)} = -\frac{\hbar^2}{2}\nabla\frac{1}{m_e}\nabla + \Delta V_e. \tag{28}$$

The solution of Eq. (27) in the spherical coordinate system is sought in the form

$$\psi_{n0}^{(i)}(r,\theta,\varphi) = R_{n0}^{(i)}(r)\, Y_{lm}(\theta,\varphi). \tag{29}$$

The radial functions $R_{n0}^{(i)}(r) = \frac{\chi_{n0}^{(i)}(r)}{r}$ are expressed in terms of the spherical Bessel functions as follows [17]:

$$\chi_{n0}^{(1)}(r) = A\, j_l(k_{1e}r) + B n_l(k_{1e}r),\ 0 \le r \le R_0, \tag{30}$$

$$\chi_{n0}^{(2)}(r) = C\, h_l^{(1)}(ik_{2e}r) + D h_l^{(2)}(ik_{2e}r),\ R_0 \le r \le R_1, \tag{31}$$

where

$$k_{1e}^2(r) = \frac{2m_1}{\hbar^2}\left(-a_c^{(1)}(\varepsilon_{\rm mech}^{(1)}(r) + \varepsilon_{\rm el-def}^{(1)}(r)\right) + \\ + e\phi^{(1)}(r) - E_{n0}),$$

$$k_{2e}^2(r) = \frac{2m_2}{\hbar^2}(\Delta E_c(0) + a_c^{(2)}(\varepsilon_{\rm mech}^{(2)}(r) + \varepsilon_{\rm el-def}^{(2)}(r)) - \\ - e\phi^{(2)}(r) - E_{n0}).$$

Using the continuity conditions for the wave function and the probability density flow across the QD-matrix interface,

$$\begin{cases} R_{1nl}(r)\big|_{r=R_0} = R_{2nl}(r)\big|_{r=R_0}, \\ \dfrac{1}{m_1}\dfrac{dR_{1nl}(r)}{dr}\Big|_{r=R_0} = \dfrac{1}{m_2}\dfrac{dR_{2nl}(r)}{dr}\Big|_{r=R_0}, \end{cases}$$

the regularity conditions for the functions $R_{nl}^{(i)}(r)$ as $r \to 0$ and $r \to R_0$, and taking the normalization condition into account, we determine the ground-state energy E_{n0} of an electron in a spherical QD from the transcendental equation

$$\frac{m_2^{(e)}}{m_1^{(e)}}\left[1 - k_{1e}R_0\ \mathrm{ctg}\,(k_{1e}R_0)\right] = \\ = \frac{1 + k_{2e}R_0 + e^{2k_{2e}(R_0-R_1)}(k_{2e}R_0 - 1)}{1 - e^{2k_{2e}(R_0-R_1)}}. \tag{32}$$

Hence, Eq. (26) averaged over the wave functions (29) reads

$$\hat{H}^{(\ln)} = E_{n0} + \sum \hbar\omega_q a_q^+ a_q + \\ + e\sqrt{\frac{2\pi\hbar}{V\varepsilon\varepsilon_0}}\sum_q \frac{\sqrt[q]{\omega_q}}{q}\left(\rho_{\ln}(q)a_q + \rho_{\ln}^*(q)a_q^+\right), \tag{33}$$

where

$$\rho_{\ln}(q) = \int e^{i\mathbf{qr}}\psi_{n0}^2(\mathbf{r})d^3r, \tag{34}$$

is the Fourier component of the electron density of states at the ln-level. By applying the unitary transformation

$$U_{\ln} = \exp\left[\sum_q \frac{e}{q}\sqrt{\frac{2\pi\hbar}{V\varepsilon_d^{(i)}\varepsilon_0\hbar\omega_q}}(\rho_{\ln}(q)a_q^+ - \rho_{\ln}^*(q)a_q)\right] \tag{35}$$

to Eq. (33), we obtain

$$\hat{H}^{(\ln)} = E_{n0} - \frac{2\pi e^2}{V\varepsilon_d^{(i)}\varepsilon_0}\sum_q \frac{|\rho_{\ln}(q)|^2}{q} + \sum_q \hbar\omega_q a_q^+ a_q. \tag{36}$$

The second term on the right-hand side of Eq. (36) is the binding energy $\Delta E^{(\ln)}$ of the electron-deformation polaron at the ln-level in the strained nanoheterosystem with the QD. Therefore, by substituting the quantity $\rho_{\ln}(q)$ from Eq. (34) into Eq. (36) and changing from summation to integration over q, we obtain

$$\Delta E^{(ln)} = -\frac{e^2}{2\varepsilon_d^{(i)}\varepsilon_0}\int \frac{\left(\psi_{n0}^{(i)}(\mathbf{r})\right)^2\left(\psi_{n0}^{(i)}(\mathbf{r}')\right)^2}{|\mathbf{r}-\mathbf{r}'|}d^3r d^3r', \tag{37}$$

where $\psi_{n0}^{(i)}(\mathbf{r})$ is the wave functions of an electron in the strained nanoheterosystem with the deformed QD [see Eq. (29)].

4. Results of Calculations and Their Analysis

The calculations were carried out for the InAs/GaAs nanoheterosystem with the following parameters: $R_0 = 100$ Å, $R_1 = 500$ Å, $a_c^{(1)} = -5.08$ eV, $a_c^{(2)} = -7.17$ eV, $a^{(1)} = 6.08$ Å, $a^{(2)} = 5.65$ Å, $m^{(1)} = 0.057m_0$, $m^{(2)} = 0.065m_0$, $\alpha = 0.657$ H/m, $n_0 = 10^{18}$ cm^{-3}, $\Delta E_c(0) = 0.83$ eV [18–20]. The energy in the potential well was reckoned from the top of the electron-deformation potential well bottom.

Figure 1 exhibits the results of numerical calculations illustrating the dependence of the potential well depth for an electron in the strained QD on the QD size, $\Delta V_c(R_0)$. The calculations were carried out with regard for the contributions from the electrostatic energy and the energy associated with the deformation of the QD and matrix materials. As one can see, the depth of the quantizing potential for the electron monotonically increases with the growth of the QD size R_0, irrespective of whether only the mechanical component of the electron-deformation potential is taken into account or together with the electrostatic potential. In particular, at the concentration of conduction electrons in the nanoheterosystem matrix $n_0 = 10^{18}$ cm^{-3} and the surface concentration of quantum dots $N_{\rm QD} = 5.5 \times 10^{10}$ cm^{-2}, the potential well depth amounts to 0.64 eV at $R_0 = 45$ Å and 0.682 eV at $R_0 = 100$ Å if the both components are considered. If the electrostatic potential is neglected, the corresponding depth values are 0.671 and 0.689 eV. The decrease in the quantizing potential depth (dashed curve *2* in Fig. 1) is stimulated by the electrostatic energy and the action of an additional compression of the QD material, which arises due to the self-consistent electron-deformation component $\varepsilon^{(i)}_{\rm el-def}(r)$ depending on the QD size R_0, the filling degree n_0 of the conduction band in the matrix, and the surface concentration of quantum dots $N_{\rm QD}$.

The compressive deformation occurring in the material of the InAs quantum dot due to the combined action of the mechanical and electron-deformation components results in a higher localization of charged quasiparticles in this QD and in a significant growth of the interaction between quasiparticles themselves and between quasiparticles and longitudinal optical phonons. In both cases, the polaron effects become stronger.

In Fig. 2, the dependences of the binding energy for an electron polaron in the ground state on the QD radius for the unstrained QD (curve *1*), the mechanically deformed QD (curve *2*), and the QD deformed by both the mechanical, $\varepsilon^{(i)}_{\rm mech}(r)$, and electron-deformation, $\varepsilon^{(i)}_{\rm el-def}(r)$, components (curve *3*) are depicted. From this figure, one can see that the binding energy of an electron polaron increases with a reduction of the QD radius in all three cases (with and without QD deformation in the strained InAs/GaAs nanoheterosystem). In particular, at $R_0 = 45$ Å, the binding energy of an electron polaron amounts to

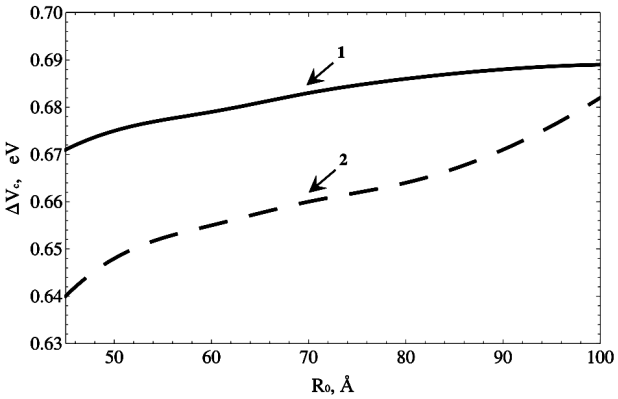

Fig. 1. Dependences of the electron potential well depth in a strained spherical QD on the QD radius R_0: only the mechanical component of the electron-deformation potential is taken into account (*1*), both the electron-deformation and electrostatic potentials are made allowance for (*2*)

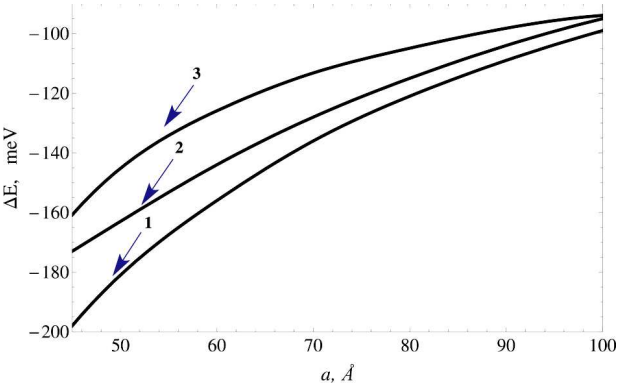

Fig. 2. Binding energy of an electron polaron in the strained InAs/GaAs nanoheterosystem: in the unstrained QD (*1*), in the strained QD if only the mechanical component of the electron-deformation potential is taken into account (*2*), in the strained QD if both the electron-deformation and electrostatic potentials are made allowance for (*3*)

−199 meV in the unstrained QD, to −174 meV in the strained QD if only the mechanical component of deformation potential is made allowance for, and to −160.8 meV in the strained QD if both the electron-deformation and electrostatic potentials are taken into consideration.

Hence, the deformation of the QD and matrix materials gives rise to higher binding energies of an electron polaron. With a reduction of the QD radius, the influence of both the mechanical and electron-deformation components becomes stronger. As the QD size R_0 increases, the binding energy of an electron-deformation polaron asymptotically approaches the binding energy of an electron polaron in the unstrained QD, because the deformation in the material decreases.

5. Conclusions

1. The theory of electron polaron states in a strained QD is developed. It involves both the mechanical and electron-deformation components of the electron-deformation potential.

2. Both the mechanical and electron-deformation components of the electron-deformation potential are found to enhance the binding energy of an electron polaron. For smaller QDs, the influence of a deformation in the QD material becomes stronger.

3. It is shown that the electron component of the electron-deformation potential and the component of the electrostatic energy, which arise due to deformations of the QD and matrix materials and the redistribution of charge carriers in a vicinity of the strained QD-matrix interface, increase the binding energy of an electron polaron. In particular, in a 45-Å quantum dot (InAs/GaAs), the electron-deformation component of the QD deformation potential increases the binding energy of the electron polaron in comparison with the binding energy of the electron polaron in a deformed QD by 12.4 meV if only the mechanical component of the deformation potential is taken into account, and by 37 meV in comparison with that in the undeformed QD.

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Received 11.06.17.
Translated from Ukrainian by O.I. Voitenko

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ПОЛЯРОННИЙ СТАН В САМОУЗГОДЖЕНОМУ ЕЛЕКТРОН-ДЕФОРМАЦІЙНОМУ ПОЛІ КВАНТОВА ТОЧКА–МАТРИЦЯ

Р е з ю м е

У межах самоузгодженої електрон-деформаційної моделі розраховано глибину потенціальної ями для електрона в наногетеросистемі з квантовими точками. Показано, що в напруженій наногетеросистемі InAs/GaAs із сферичними квантовими точками InAs існують деформаційні поля, які виникають на межі розподілу квантова точка–матриця, що приводять до підсилення поляронних ефектів порівняно з недеформованими матеріалами. Розраховано енергію електронного полярона із врахуванням внесків електростатичної енергії та енергії, зумовленої як механічною, так і електрон-деформаційною складовими деформацій матеріалів КТ та матриці.