Condensed Matter Physics 2009, Vol. 12, No 2, pp. 215–223

CONDENSED MATTER PHYSICS

# Electric properties of the interface quantum dot – matrix

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Received March 31, 2009, in final form May 13, 2009

A theoretical research is presented concerning the potential distribution and electric field intensity in the InAs/GaAs nanoheterosystem with InAs QDs within the framework of self-consistent electron-deformation model. It is shown that at the strained border between a quantum dot and matrix there is a double electric layer, that is $n^{+} - n$ junction.

**Key words:** *quantum dots, electron-deformation and electrostatic potentials*

**PACS:** *68.65.Hb, 73.21.La, 73.63.Kv*

## 1. Introduction

At present, the study of electric properties of stressed heteroborder between a quantum dot(QD) (InAs, CdTe) and matrix (GaAs, ZnTe) is of great interest [1]. This interest is related to the development of new approaches to the creation of p-n structures on QDs, specifically tunnel diodes [2], quantum transistors [3], elements of one-electronic memory [4]. Stresses that arise in nanoheterosystems with QDs both in the process of growth and temperature changes, and during fabrication on their basis of opto- and nanoelectronics devices, effect the shape and the potential barrier height at the border between a QD and a matrix, the band-gap energy, a discrete spectrum of energy states of the electrons localised in a QD, the charge emission from the QD into the corresponding bands of the semiconductor, the barrier capacity of the structure and the width of the space charge region.

Electrical and optical properties of nanoheterostructures with QDs are defined, mainly, by an energy distribution of charge carriers. Therefore, such properties should be sensitive to the sizes, to the shape, to the composition of nanocluster InAs(CdTe) and strains of materials of nanocluster and the surrounding matrix GaAs(ZnTe), since deformation effects the depth and the character of quantizing potential of a quantum dot. In particular,nanoclusters InAs (CdTe) create in matrix GaAs (ZnTe) the potential wells for electrons and holes, which can be negatively or positively charged, capturing electrons and holes from the surrounding volume of a matrix. The degree of charging of a QD by carriers and their emission will depend on the character and size of deformation of nanocluster and matrices materials, which effects both the energy location of local levels in a QD and the location of electrochemical potential in a nanoheterostructure.

In papers [5,6], the authors have explored, for the one-dimensional case, a potential distribution in the field of a spatial charge in the vicinity of the boundary of the contact between metal and semiconductor GaAs with a layer of quantum dots InAs [5], capacitance-voltage characteristics [5], potential distribution and transport processes in silicon Shottki diodes, which contain an array of germanium nanoclusters [6]. Theoretical research in articles [5,6] was done without taking into account the deformation effects, which essentially effect the transport properties of the carriers in nanoheterosystems with quantum dots.

The purpose of the given paper is to study the potential distribution and electric field at the strained boundary between a QD (InAs, CdTe) and the matrix (GaAs, ZnTe) within the framework of self-consistent electron-deformation model [7]. Thus, knowing the mechanism of changing the character of a potential distribution and an electric field in nanoheterosystem with an array of quantum dots, under the effect of deformation fields, it is possible to predict and control electrical properties of p–n structures, which are created on the basis of strained nanoheterosystems with an array of QDs.

## 2. Model of the potential and electric field distribution in a spherical QD InAs and in the matrix GaAs

In this formulation of the problem, nanoheterosystems InAs/GaAs (001) with coherently strained InAs quantum dots without a precisely determined crystallographic facet are considered. Technologically, such QDs can be obtained if the thickness of the InAs growing layer becomes of the order of 2 monolayers (ML) [8]. Therefore, in what follows, both the contribution of the island edges to the elastic deformation energy and, correspondingly, the jump of the strain tensor at the island edges can be neglected.

We consider the InAs/GaAs heterosystem with coherently stressed spherical InAs QDs. In order to reduce the problem with a large number of QDs to the problem with one QD, we use the following approximation. The energy of the pairwise elastic interaction between the QDs can be replaced by the energy of interaction of each QD with the averaged elastic strain field $\sigma_{\mathrm{ef}}(N-1)$ of all other $(N-1)$ QDs [9]. Thus, QD InAs in matrix n-GaAs creates a potential well for electrons, and in p-GaAs – a potential well for holes, accordingly (see figure 1). The given potential wells can be charged with the negative or positive charge.

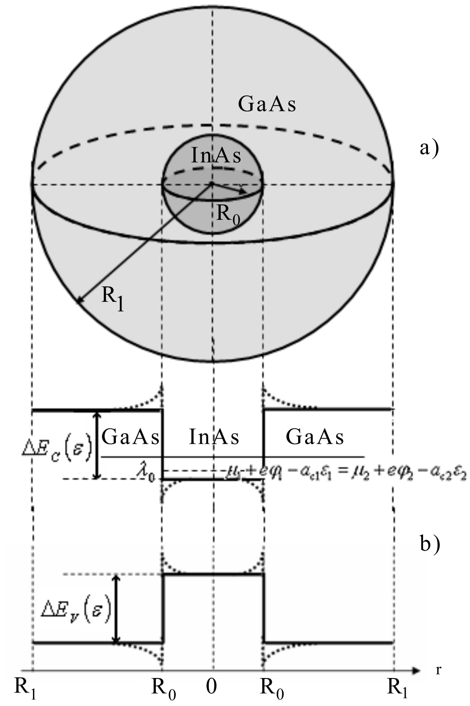


**Figure 1.** Geometry model (a) and zone scheme (b) of a InAs/GaAs nanoheterosystem with InAs QDs (solid line without taking into account deformation effects, dashed line -with deformation effects).

Under the effect of inhomogeneous deformation of compression of QD InAs material and inhomogeneous deformation of tension of matrix GaAs material, which surrounds a quantum dot, the band structure of the nanoheterosystem with QDs locally changes (see figure 1b). Such a change, as a result of self-compounding of an electron-deformation framework, leads to redistribution of electronic density in the surroundings of strained boundary between a quantum dot and matrix. Therefore, in the material of a QD, near heteroboundary, there is a surplus of negative charge while in the matrix material there is a shortage. Thus, at the strained heteroboundary between a quantum dot and the matrix there arises $n^{+}-n$ junction (electron-deformation dipole $\vec{P}_{\text{el.}-\text{def.}}$).

The mathematical model featuring a potential distribution at the strained heteroboundary between QD and matrix consists of the following self-compounded combined equations:
*the Schrodinger equation*

$$\left[\frac{\hbar^2}{2m_i^*}\Delta_{\vec{r}}+V_{\text{def}}^{(i)}(\vec{r})-\mathrm{e}\varphi_i(\vec{r})\right]\psi_n^{(i)}(\vec{r})=\tilde{E}_n\psi_n^{(i)}(\vec{r}),\qquad i=\begin{cases}1\equiv\text{InAs},\\2\equiv\text{GaAs},\end{cases}\tag{1}$$

$$V_{\text{def}}^{(i)}(\vec{r})=\begin{cases}-\left(|\Delta E_c|-\left|a_c^{(1)}\varepsilon_1\right|-\left|a_c^{(2)}\varepsilon_2\right|\right),\\0.\end{cases}\tag{2}$$

here $\Delta E_c$ – is the depth of the potential well for electrons in the QD in a non-deformed heterostructure InAs/GaAs; $\tilde{E}_n=E_n-\lambda_0$ is eigenvalues Schrodinger functional; $\lambda_0$ is the energy of the bottom of non-deformed allowed band; $a_c^{(i)}$ – is the constant of the hydrostatic deformation potential of the conduction band; $\varepsilon_i(\vec{r})=\mathrm{Sp}\,\hat{\varepsilon}_i$ is deformation parameter, which is defined through displacement of atoms $\vec{u}_i$, which are taken from the equilibrium equation:

$$\vec{\nabla}\mathrm{div}\vec{u}_i=-D^{(i)}\cdot\vec{F}^{(i)}\left(\vec{r}\right),\tag{3}$$

where $\vec{F}^{(i)}(\vec{r})=-\mathrm{e}\delta\vec{E}^{(i)}, D^{(i)}=\frac{(1+\nu_i)\,(1-2\nu_i)}{(a^{(i)})^3E_i\,(1-\nu_i)}$ here $\delta\,\vec{E}$ is redundant electric field, which arises at the strained interface between quantum dot and matrix, the intensity of which is determined through a gradient of electrostatic potential $\left(\delta E^{(i)}=-\frac{\mathrm{d}\varphi^{(i)}(\vec{r})}{\mathrm{d}r}\right)$; $a^{(i)}$ is lattice parameter; $\nu_i$ are Poisson coefficients; $E_i$ is Young modulus of the QD and surrounding matrix materials; $e$ is elementary electronic charge.

From the Poisson equation we find electrostatic potential $\varphi^{(i)}\left(\vec{r}\right)$:

$$\Delta\varphi_i(\vec{r})=\frac{\mathrm{e}}{\varepsilon_{\mathrm{d}}^{(i)}\varepsilon_0}\Delta n_i(\vec{r}),\tag{4}$$

where $\varepsilon_{\mathrm{d}}^{(i)}$ is relative dielectric constant; $\Delta n_i(\vec{r})$ is the change of electron density at the interface between QD and matrix and can be obtained through superposition of wave function multiplication, which are solutions of the Schrodinger equation(1):

$$n_i(r)=\sum_n\frac{\psi_n^{*(i)}(\vec{r})\psi_n^{(i)}(\vec{r})}{\exp(\beta(\tilde{E}_n-\mu_i))+1}\,,\tag{5}$$

where $\mu_i$ is chemical potential; and equation for defining the electrochemical potential:

$$\frac{1}{\Omega_0}\int n(\vec{r})\mathrm{d}\vec{r}=n_0\,,\tag{6}$$

here $\Omega_0$ is the volume of unit cell, $n_0$ is the average electron density in nanoheterostructure with QDs.

Since in the task there is considered a spherically – symmetrical nanoheterosystem, the system of equations (1)–(6) will take the following form:

$$\left[-\frac{\hbar^2}{2m_i^*}\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{2}{r}\frac{\mathrm{d}}{\mathrm{d}r}-\frac{l(l+1)}{r^2}\right)+V_{\text{def}}^{(i)}(r)-\mathrm{e}\varphi_i(r)\right]R_{\text{nl}}^{(i)}(r)=E_{n_r}R_{\text{nl}}^{(i)}(r)\,,\tag{7}$$

where $R_{\text{nl}}^{(i)}(r)$ is radial wave function of electrons. Radial wave functions $R_{\text{nl}}^{(i)}$ are the solutions of the radial Schrodinger equation(7) with deformation potential(2):

$$\begin{aligned}R_{\text{nl}}^{(1)}(r)&=Aj_l(k_{\text{nl}}r)+Bn_l(k_{\text{nl}}r),\qquad 0\leqslant r\leqslant R_0\,,\\R_{\text{nl}}^{(2)}(r)&=Ch_l^{(1)}(i\chi_{\text{nl}}r)+Dh_l^{(2)}(i\chi_{\text{nl}}r)\,,\qquad R_0\leqslant r\leqslant R_1\,,\end{aligned}\tag{8}$$

where

$$k_{\rm nl}^2 = \frac{2m_1^*}{\hbar^2}\left(\left|V_{\rm def}^{(1)}\right| - |E_{\rm nl}|\right),$$
$$\chi_{\rm nl}^2 = \frac{2m_2^*}{\hbar^2}|E_{\rm nl}|\,. \tag{9}$$

The continuity conditions for the wave functions and density of the flow of probability at the QD-matrix interface,

$$\begin{cases} R_{\rm nl}^{(1)}(r)\,|_{r=R_0} = R_{\rm nl}^{(2)}(r)\,|_{r=R_0}, \\ \frac{1}{m_1^*}\frac{{\rm d}R_{\rm nl}^{(1)}(r)}{{\rm d}r}\,|_{r=R_0} = \frac{1}{m_2^*}\frac{dR_{\rm nl}^{(2)}(r)}{dr}\,|_{r=R_0} \end{cases} \tag{10}$$

along with the regularity condition of the function $R_{\rm nl}^{(1)}(r)$ at $r \to 0$, zero equality of the function $R_{\rm nl}^{(2)}(r)$ at $r \to R_1$ $\left(R_{\rm nl}^{(2)}(r)\,|_{r=R_1} = 0\right)$ and with normalization, determine the energy spectrum $E_{\rm nl}$ and wave functions of the electron in the InAs/GaAs heterosystem with the InAs QD. Therefore, the energy of the ground state of the electron in the QD is determined from the following transcendental equation[9]:

$$k\,{\rm tg}\left(kR_0 - n\frac{\pi}{2}\right) = \chi\frac{m_1^*}{m_2^*}{\rm ctgh}(\chi(R_1 - R_0)) + \frac{m_1^* - m_2^*}{R_0\,m_2^*}, \qquad n = 1. \tag{11}$$

In case of spherical symmetry, the equilibrium equation(3) can be presented in the form:

$$\frac{{\rm d}^2u_r^{(i)}}{{\rm d}r^2} + \frac{2}{r}\frac{{\rm d}u_r^{(i)}}{{\rm d}r} - \frac{2}{r^2}u_r^{(i)} = D^{(i)}{\rm e}\,\frac{{\rm d}\varphi^{(i)}(r)}{{\rm d}r} \tag{12}$$

here $u_r^{(i)}$ is radial component of displacements of atoms. General solution of the heterogeneous equation(12) is presented in the form of the sum of mechanical $u_{r\,{\rm mech}}^{(i)}(r)$ and electron-deformation $u_{\rm rel-def}^{(i)}(r)$ displacements components:

$$u_r^{(i)}(r) = u_{r\,{\rm mech}}^{(i)}(r) + u_{\rm rel-def}^{(i)}(r), \tag{13}$$

where $u_{r\,{\rm mech}}^{(i)}(r) = C_1^{(i)}r + \frac{C_2^{(i)}}{r^2}$, $u_{\rm rel-def}^{(i)}(r) = -\frac{D^{(i)}e}{r^2}\int r^2\varphi^{(i)}(r)\,{\rm d}r$. For insignificant conduction electron concentrations in a matrix of the nanoheterosystem (n0 $< 10^{18}$ sm$^{-3}$), the value of the electron-deformation component of displacements $u_{\rm rel-def}^{(i)}(r)$ in QD is one order smaller than the mechanical component of displacements $u_{r\,{\rm mech}}^{(i)}(r)$. Therefore, in the first approximation we ignore the electron-deformation component of displacements $u_{\rm rel-def}^{(i)}(r)$

The field of displacements determines the following components of the strain tensor:

$$\varepsilon_{rr}^{(1)} = \varepsilon_{\varphi\varphi}^{(1)} = \varepsilon_{\theta\theta}^{(1)} = C_1^{(1)}, \tag{14}$$

$$\varepsilon_{rr}^{(2)} = C_1^{(2)} - \frac{2C_2^{(2)}}{r^3}, \tag{15}$$

$$\varepsilon_{\varphi\varphi}^{(2)} = \varepsilon_{\theta\theta}^{(2)} = C_1^{(2)} + \frac{C_2^{(2)}}{r^3}\,. \tag{16}$$

The coefficients $C_1^{(1)}, C_1^{(2)}, C_2^{(2)}$ are determined from the solution of the following combined equations :

$$\begin{cases} u_r^{(2)}|_{r=R_0} - u_r^{(1)}|_{r=R_0} = fR_0, \\ \sigma_{rr}^{(1)}|_{r=R_0} = \sigma_{rr}^{(2}|_{r=R_0} + P_L|_{r=R_0}, \qquad P_L = \frac{2\alpha}{R_0 - \left|u_r^{(1)}\right|}, \\ \sigma_{rr}^{(2)}|_{r=R_1} = -\sigma_{\rm ef}(N-1), \end{cases} \tag{17}$$

$\alpha$ – is the surface energy of the InAs QD [10], $f$ – is the lattice mismatch of the materials of the QD and the matrix:$f = \frac{a^{(1)}-a^{(2)}}{a^{(1)}} \approx 7\%$ ; $\sigma_{rr}^{(i)}$ are radial components of the mechanical strain tensor [11].

Poisson equation(4) can be presented in the form:

$$\frac{\mathrm{d}^2\varphi^{(i)}}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}\varphi^{(i)}}{\mathrm{d}r} = \frac{\mathrm{e}}{\varepsilon_{\mathrm{d}}^{(i)}\varepsilon_0}\left(n_i(r) - n_0\right). \tag{18}$$

The charge density in a strained nanoheterostructure with a quantum dot was calculated with $\delta$ – similar density of electronic state in QD $\delta\left(E' - E_n\right) \approx \frac{1}{\sqrt{\pi/2}\,\Delta E}\exp\left(\frac{-2\left(E'-E_n\right)^2}{\Delta E^2}\right)$. Specifically, at the $T = 0\,K$ temperature in the QD ($0 \leqslant r \leqslant R_0$) and matrix ($R_0 \leqslant r \leqslant R_1$), the charge density $n_i(r)$ can be obtained from the following formula :

$$\begin{aligned} n_i\left(r\right) &= \int_0^{\mu-\lambda_0^{(i)}-a_c^{(i)}\varepsilon_{rr}^{(i)}+\mathrm{e}\varphi_i(r)} \frac{2N_{\mathrm{QD}}}{a^{(i)}\sqrt{\pi/2}\,\Delta E}\,\mathrm{e}^{\frac{-2\left(E'-E_1\right)^2}{\Delta E^2}}\left|\psi_{nlm}^{(i)}\right|^2\mathrm{d}E' \\ &= \left|\psi_{nlm}^{(i)}\right|^2\frac{N_{\mathrm{QD}}}{a^{(i)}}\left(\mathrm{erf}\left(\frac{\sqrt{2}}{\Delta E}E_1\right) + \mathrm{erf}\frac{\sqrt{2}}{\Delta E}\left(\mu - E_1 - \lambda_0^{(i)} - a_c^{(i)}\varepsilon_{rr}^{(i)} + \mathrm{e}\varphi_i\left(r\right)\right)\right), \end{aligned} \tag{19}$$

where $N_{\mathrm{QD}}$ surface density of quantum dots, which is equal in nanoheterostructure InAs/GaAs with QDs InAs $\approx 3\times10^{10}\ \mathrm{sm}^{-2}$ [12]; $\Delta E$ – half-width of Gauss line;$E_1$ – energy of an electron at the first localized level in a quantum well; $\psi_{nlm}^{(i)}\left(r,\theta,\varphi\right) = R_{\mathrm{nl}}^{(i)}(r)\cdot Y_{lm}(\theta,\varphi)$ – the solution of the Schrodinger equation (1) in the spherical system of coordinates; $Y_{lm}(\theta,\varphi)$ – the spherical Legendre functions [13].

The Poisson equation (18) concentration of charge carriers $n_i(r)$(19) is a nonlinear function from $\varphi_i(r)$. Therefore, first of all we linearize it, i. e., we substitute Taylor expansion for expression (18) in the Poisson equation:

$$\begin{aligned} n_i(r) \approx\ & \left|\psi_{nlm}^{(i)}\right|^2\frac{N_{\mathrm{QD}}}{a^{(i)}}\left[\mathrm{erf}\left(\frac{\sqrt{2}}{\Delta E}E_1\right) + \mathrm{erf}\left(\frac{\sqrt{2}}{\Delta E}\left(\mu - E_1 - \lambda_0^{(i)} - a_c^{(i)}\varepsilon_{rr}^{(i)}\right)\right)\right. \\ & \left. + \sqrt{\frac{8}{\pi}}\frac{e}{\Delta E}\mathrm{e}^{\frac{-2\left(\mu-E_1-\lambda_0^{(i)}-a_c^{(i)}\varepsilon_{rr}^{(i)}\right)^2}{\Delta E^2}} \times \varphi_i\left(r\right)\right]. \end{aligned} \tag{20}$$

The solution of the Poisson equation (18) in the QD and matrix, taking into account the expression for an electron concentration(20), with an average frequency function $\left|\bar{\psi}_i\right|^2$ has the following form:

$$\varphi_1(r) = A_1\frac{\sinh\left(\sqrt{\frac{1}{a_1}}r\right)}{r} - a_1 b_1\,, \tag{21}$$

$$\begin{aligned} \varphi_2(r) =\ & B_1\frac{\exp\left(-\sqrt{\frac{1}{a_2}}r\right)}{r} + B_2\frac{\exp\left(\sqrt{\frac{1}{a_2}}r\right)}{r} - a_2 b_2 - \frac{d_2}{2r} \\ & \times\left[\exp\left(-\sqrt{\frac{1}{a_2}}r\right)\times Ei\left(\sqrt{\frac{1}{a_2}}r\right) + \exp\left(\sqrt{\frac{1}{a_2}}r\right)\times Ei\left(-\sqrt{\frac{1}{a_2}}r\right)\right], \end{aligned} \tag{22}$$

where

$$Ei\left(z\right) = -\int_{-z}^{\infty}\frac{\exp\left(-t\right)}{t}\mathrm{d}t,$$

$$\frac{1}{a_1} = \frac{\mathrm{e}^2}{\varepsilon_{\mathrm{d}}^{(1)}\varepsilon_0 a^{(1)}}\left|\bar{\psi}_1\right|^2 N_{\mathrm{QD}}\frac{\sqrt{\frac{8}{\pi}}}{\Delta E}\exp\left(\frac{-2\left(\mu - E_1 - \lambda_0^{(1)} - a_c^{(1)}C_1^{(1)}\right)^2}{\Delta E^2}\right),$$

$$
\begin{aligned}
\frac{1}{a_2} &= \frac{\mathrm{e}^2}{\varepsilon_{\mathrm{d}}^{(2)}\varepsilon_0 a^{(2)}}\left|\bar{\psi}_2\right|^2 N_{\mathrm{QD}}\frac{\sqrt{\frac{8}{\pi}}}{\Delta E}\exp\left(\frac{-2\left(\mu-E_1-\lambda_0^{(2)}-a_c^{(2)}C_1^{(2)}\right)^2}{\Delta E^2}\right),\\
d_2 &= \frac{2a_c^{(2)}C_2^{(2)}e}{\varepsilon_{\mathrm{d}}^{(2)}\varepsilon_0 a^{(2)}}\left|\bar{\psi}_2\right|^2 N_{\mathrm{QD}}\frac{\sqrt{\frac{8}{\pi}}}{\Delta E}\exp\left(\frac{-2\left(\mu-E_1-\lambda_0^{(2)}-a_c^{(2)}C_1^{(2)}\right)^2}{\Delta E^2}\right),\\
b_1 &= \frac{\mathrm{e}}{\varepsilon_{\mathrm{d}}^{(1)}\varepsilon_0 a^{(1)}}\left|\bar{\psi}_1\right|^2 N_{\mathrm{QD}}\left[\operatorname{erf}\left(\frac{\sqrt{2}}{\Delta E}E_1\right)+\operatorname{erf}\left(\frac{\sqrt{2}}{\Delta E}\left(\mu-E_1-\lambda_0^{(1)}-a_c^{(1)}C_1^{(1)}\right)\right)\right.\\
&\quad\left.-\frac{a^{(1)}n_0}{\left|\bar{\psi}_1\right|^2 N_{\mathrm{QD}}}\right],\\
b_2 &= \frac{\mathrm{e}}{\varepsilon_{\mathrm{d}}^{(2)}\varepsilon_0 a^{(2)}}\left|\bar{\psi}_2\right|^2 N_{\mathrm{QD}}\left[\operatorname{erf}\left(\frac{\sqrt{2}}{\Delta E}E_1\right)+\operatorname{erf}\left(\frac{\sqrt{2}}{\Delta E}\left(\mu-E_1-\lambda_0^{(2)}-a_c^{(2)}C_1^{(2)}\right)\right)\right.\\
&\quad\left.-\frac{a^{(2)}n_0}{\left|\bar{\psi}_2\right|^2 N_{\mathrm{QD}}}\right].
\end{aligned}
$$

Accordingly, the expression for an electric field intensity in quantum dots and a matrix will look like this:

$$
\begin{aligned}
E_1(r) &= A_1\frac{\sqrt{\frac{1}{a_1}}r\cosh\left(\sqrt{\frac{1}{a_1}}r\right)-\sinh\left(\sqrt{\frac{1}{a_1}}r\right)}{r^2}, && (23)\\
E_2(r) &= -\frac{d_2}{r^2}+\frac{\mathrm{e}^{-\sqrt{\frac{1}{a_2}}r}}{r}\left(\frac{d_2}{2}Ei\left(\sqrt{\frac{1}{a_2}}r\right)-B_1\right)\left(\frac{1}{r}+\sqrt{\frac{1}{a_2}}\right)\\
&\quad+\frac{\mathrm{e}^{\sqrt{\frac{1}{a_2}}r}}{r}\left(\frac{d_2}{2}Ei\left(-\sqrt{\frac{1}{a_2}}r\right)-B_2\right)\left(\frac{1}{r}-\sqrt{\frac{1}{a_2}}\right). && (24)
\end{aligned}
$$

The coefficients $A_1, B_1, B_2$ in expressions (21)–(24) are determined from requirements of a continuity of potentials $\varphi_1(r)$ and $\varphi_2(r)$ at the strained heteroboundary, normal component of a vector of an electric displacement and the condition of neutrality.

$$
\begin{cases}
\varphi^{(1)}(r)|_{r=R_0}=\varphi^{(2)}(r)|_{r=R_0}\,,\\
\varepsilon_1\frac{d\varphi^{(1)}(r)}{dr}|_{r=R_0}=\varepsilon_2\frac{d\varphi^{(2)}(r)}{dr}|_{r=R_0}\,,\\
\int\limits_0^{R_0} r^2\Delta n_1(r)\mathrm{d}r+\int\limits_{R_0}^{R_1} r^2\Delta n_2(r)\mathrm{d}r=0.
\end{cases} \qquad (25)
$$

## 3. Numerical calculations and discussion of results

Further, we present the results of theoretical research of the dependence of the electrostatic potential and electric field intensity in the InAs QD and in the matrix within the framework of self-consistent electron-deformation model. The calculations were performed for the following parameters ([10,14,15]): $a^{(1)}=6.08$ Å; $a^{(2)}=5.65$ Å; $C_{11}^{(1)}=0.833$ Mbar; $C_{12}^{(1)}=0.453$ Mbar; $C_{11}^{(2)}=1.223$ Mbar; $C_{12}^{(2)}=0.571$ Mbar; $\Delta E_c(0)=0.83$ eV; $a_c^{(1)}=-5.08$ eV; $a_c^{(2)}=-7.17$ eV; $E_g^{(1)}(0)=0.36$ eV; $E_g^{(2)}(0)=1.452$ eV; $R_1=1000$ Å; $\sigma_{\mathrm{ef}}=10^9 N/m^2$; $m_1^{(\mathrm{e})}=0.057m_0$; $m_2^{(\mathrm{e})}=0.065m_0$; $\alpha=0.657$ H/m.

Figure 2–4 shows the dependence of electrostatic potential $\varphi(r)$ (figure 2), electric field intensity (figure 3) and charge density $\Delta n(r)$ (figure 4) in a InAs/GaAs nanoheterosystem with InAs QDs size : $R_0=50$ Å, $R_0=100$ Å.

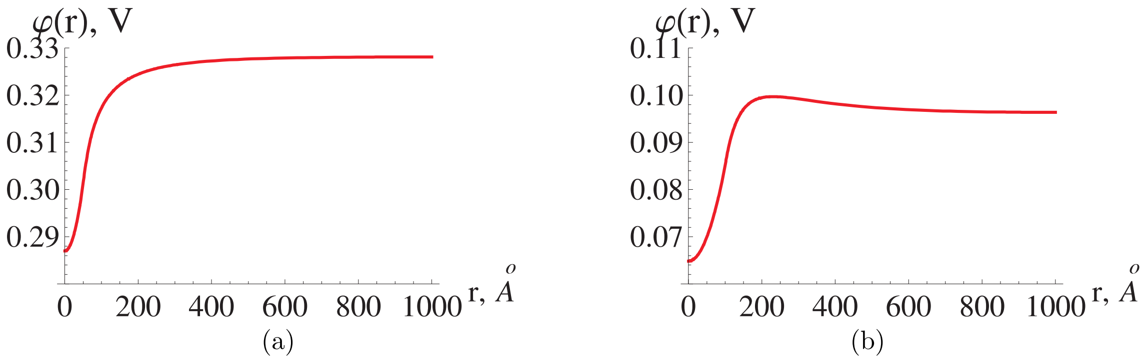


**Figure 2.** Coordinate dependence of the electrostatic potential $\varphi(r)$ in the InAs/GaAs nanoheterosystem with InAs QDs; (a) $R_0 = 50$ Å, (b) $R_0 = 100$ Å.

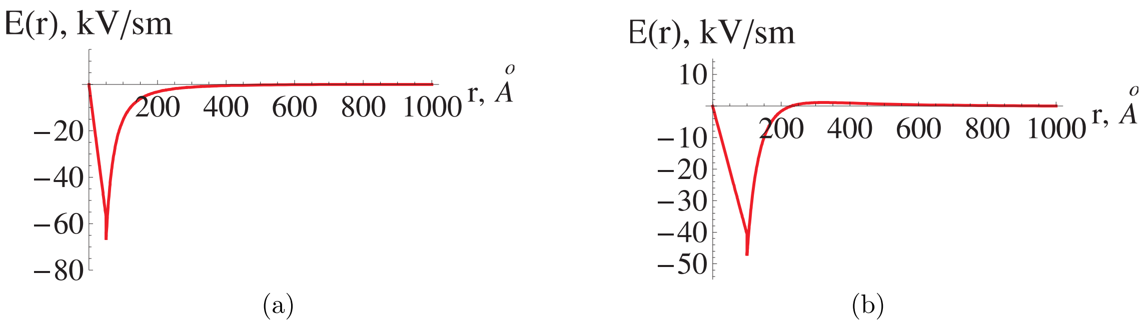


**Figure 3.** Coordinate dependence of the electric field intensity $E(r)$ in the InAs/GaAs nanoheterosystem with InAs QDs; (a) $R_0 = 50$ Å, (b) $R_0 = 100$ Å.

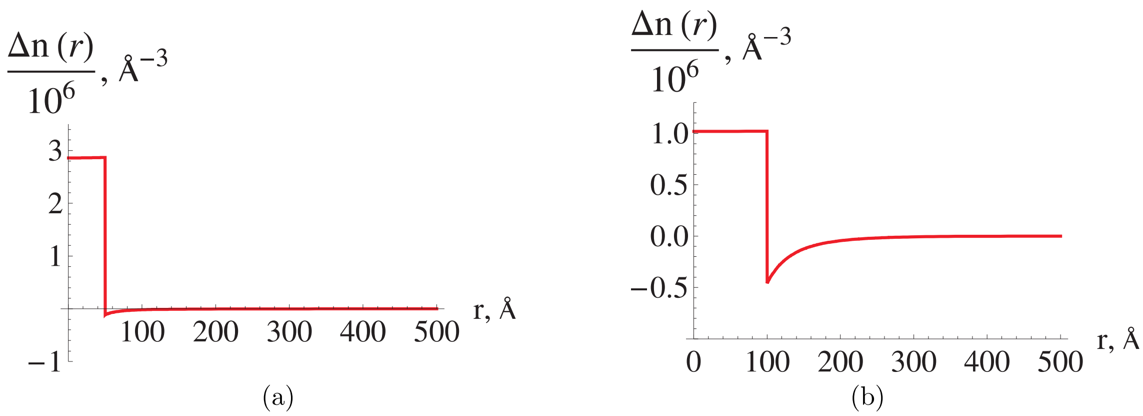


**Figure 4.** Coordinate dependence of the charge density $\Delta n(r)$ in the InAs/GaAs nanoheterosystem with InAs QDs; (a) $R_0 = 50$ Å, (b) $R_0 = 100$ Å.

It is evident from figure 2 that electrostatic potential $\varphi(r)$, in such nanoheterosystem, deflates when the size of QD increase. In particular, the increase of the QD radius $R_0$ from 50 to 100 Å results in a decrease of the electrostatic potential at the interface between QD and matrix by about 206 meV.

Potential distribution $\varphi(r)$ , in such nanoheterosystem, subject to the size of a QD has a monotonous (figure 2a) or a nonmonotonous character (figure 2b). Specifically, coordinate dependence of the electrostatic potential for QDs at the sizes 20 Å $\leqslant R_0 \leqslant$ 70 Å is monotonous, and at the sizes $R_0 > 70$ Å it is nonmonotonous, the maximum location of which is defined by radius of a QD. Such a character of electrostatic potential $\varphi(r)$ distribution in QDs of different sizes is defined by redistribution of an electronic density of charge $\Delta n = \Delta n\,(\vec{r})$ (see figure 4) at the QD – matrix interface. At the QD – matrix interface, electrostatic potential $\varphi\,(r)$ is changed and moving from boundary $(r \to R_1)$ the potential goes to the value $\varphi\,(r)\,|_{r=R_1} \approx B_2 \frac{\mathrm{e}^{\sqrt{\frac{1}{a_2}}R_1}}{R_1} - a_2 b_2$.

Figure 3 shows the electric field intensity distribution in the QD and in the matrix. As numerical calculations show the electric field intensity deflates with an increase of the QD size, and it is maximal at the QD – matrix interface. Specifically, for a QD at the size 50 Å $E(r)\,\big|_{r=R_0} = 66\frac{\mathrm{kV}}{\mathrm{sm}}$ and at the size 100 Å – $E(r)\,\big|_{r=R_0} = 49\frac{\mathrm{kV}}{\mathrm{sm}}$. The decrease of the electric field intensity when the size of QD increases is specified by a decrease of the deformation potential. With a distance from the boundary, the electric field intensity in QD wanes and is equal to zero at the center of QD, and in the matrix it has a nonmonotonous character and approaching the matrix edge it wanes to zero.

As it is shown in the figures (figures 4a,b) at the QD – matrix interface, spatial redistribution of electrons takes place: the electrons are excessive near the interface in the QD InAs(CdTe), and they are depleted in the matrix GaAs(ZnTe). The effect of electrostatic interaction of charges leads to such a redistribution of electronic density that at the strained border between quantum dot and matrix there arises a double electric layer, i. e., $n^+ - n$ junction. It is possible to control the electrical properties of $n^+ - n$ junction at the expense of the surface density$N_{\mathrm{QD}}$ variation of QDs. Observationally, it is possible to define the concentration profile of the majority carriers of a charge in such a nanoheterosystem with QDs by differentiating the C–V [16] characteristic: $n^{(i)}(r) = 2\left[\varepsilon_{\mathrm{d}}^{(i)}\varepsilon_0 S^2 \frac{\mathrm{d}}{\mathrm{d}V}\left(\frac{1}{C^2}\right)\right]^{-1}$ ($S$ are contact surfaces between a quantum dot and a matrix, $r$ is a moving coordinate of the boundary space-charge region).

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# Електричні властивості межі поділу квантова точка – матриця

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Отримано 31 березня 2009 р., в остаточному вигляді – 13 травня 2009 р.

У межах моделі самоузгодженого електрон-деформаційного зв'язку, теоретично досліджено розподіл потенціалу та напруженості електричного поля в напруженій наногетеросистемі InAs/GaAs з квантовими точкам InAs. Показано, що на напруженій межі квантова точка – матриця виникає подвійний електричний шар, тобто $n^{+}-n$ перехід.

**Ключові слова:** *квантові точки, електрон-деформаційний та електростатичний потенціали*

**PACS:** *68.65.Hb, 73.21.La, 73.63.Kv*