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# FORMATION OF $n^+ - n$ JUNCTIONS AT A STRESSED INTERFACE QUANTUM DOT–MATRIX

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The theory of the formation of  $n^+ - n$  junctions in stressed nanoheterosystems with quantum dots (QDs) has been developed in the framework of the self-consistent electron-deformation model. An electric double layer, i.e. an  $n^+ - n$  junction, has been shown to emerge at the QD–matrix stressed interface.

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cular, InAs(CdTe) nanoclusters create potential wells for electrons and holes in the GaAs(ZnTe) matrix. The wells can be charged negatively and positively due to the capture of electrons and holes, respectively, from the surrounding bulk of the matrix. The degree of charging of a QD by charge carriers and their emission depend on the character and the magnitude of deformation, which the materials of a nanocluster and the matrix are subjected to. The deformation affects both the energy positions of local levels in the QD and the position of the electrochemical potential in a nanoheterostructure.

## 1. Introduction

The last decade is characterized by a powerful development of nanoelectronics, which is associated to a great extent with the implementation of nanostructures with QDs into the fabrication of nanooptoelectronic devices. A specific place belongs to nanostructures with QDs that self-organize at heteroepitaxy of elastically stressed layers [1–3], because such QDs have small dimensions (of about 10 nm) and are characterized by small dispersions of both their dimensions and shapes. Stresses that arise in nanoheterostructures with QDs – e.g., in the course of growth processes and at temperature variation, as well as when manufacturing the devices of solid-state nanooptoelectronics on their basis (heterolasers [1], infra-red photodetectors [4], tunnel diodes [5], quantum transistors [6], single-electron memory cells [7]) – affect the shape and the height of potential barriers at the interface QD–matrix, the energy gap width, the discrete spectrum of energy states of electrons localized in a QD, the filling kinetics of a QD by charge carriers, the charge emission from a QD into the corresponding bands of a semiconductor, the barrier capacity of the structure, and the width of the space charge region.

Electrical and optical properties of nanoheterostructures with QDs are mainly governed by the energy spectrum of charge carriers. Therefore, such properties should be sensitive to the dimensions, shape, and composition of nanoclusters InAs(CdTe), and to the deformation of materials the nanocluster and the surrounding matrix GaAs(ZnTe) consist of. It is so, because a deformation influences the depth and the character of the quantizing potential of a QD. In parti-

In work [8], the potential distribution in the space charge region in the vicinity of the contact between a metal and a GaAs semiconductor with a layer of InAs quantum dots and the corresponding capacity-voltage characteristics were studied in the one-dimensional case. In work [9], in the same approximation, both the potential distribution and the transport processes in silicon Schottky diodes that contain an array of germanium nanoclusters were investigated. Theoretical researches in works [8, 9] were carried out, not taking deformation effects into account. The latter substantially affect the transport properties of charge carriers in those nanoheterosystems with QDs, because a mismatch between the corresponding lattice constants of contacting materials amounts to about 7% [3].

This work aimed at studying the potential and electron density distributions in the vicinity of the stressed interface QD (InAs, CdTe)–matrix (GaAs, ZnTe). The calculations were carried in the framework of the self-consistent electron-deformation model [10]. Knowing the regularities in a variation of the potential distribution and the redistribution of the electron concentration in the nanoheterosystem with an array of QDs, which occur under the influence of deformation fields, one can fulfill a predicted control over the electric properties of semiconductor Schottky diodes created on the basis of stressed nanoheterosystems with a QD array.

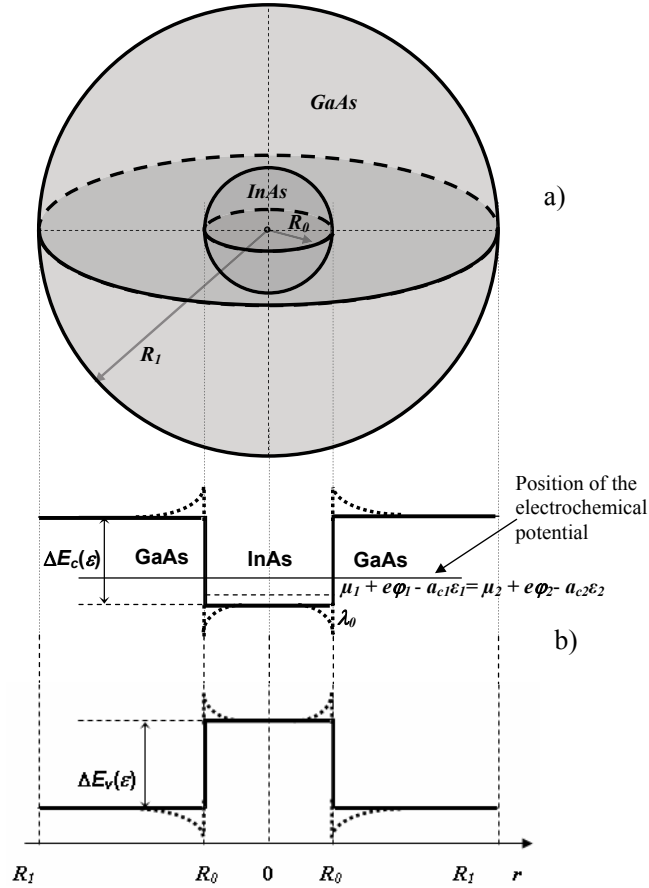


Fig. 1. Geometrical model (a) and band diagram (b) of a nanoheterosystem with a quantum dot. The dashed and the solid curve correspond to the cases, when the electron-deformation interaction is and is not taken into account

**2. Model of  $n^+ - n$  Junction Formation in a Stressed Nanoheterosystem with QDs**

In this paper, we consider QDs that have no pronounced crystallographic faceting, in particular, those, whose shape approximately corresponds to a spherical symmetry. Such a case is realized, for instance, in an InAs/GaAs (001) heterosystem with InAs quantum dots, when the thickness of the deposited InAs layer is about two monolayers [11, 12]. Therefore, we neglect the contribution of island edges to the energy of elastic relaxation.

The ordered arrangement of stressed QDs in the crystal matrix is determined by elastic interaction between islands which arises due to a mismatch between the lattice constants of InAs and GaAs ( $f \approx 7\%$ ). To reduce the problem with plenty of QDs to a problem with a single QD, we made the following approximation:

the energy of paired elastic interaction between QDs is replaced by the energy of interaction between every QD with the mean field of elastic deformation  $\sigma_{\text{eff}}(N - 1)$  of all other QDs [13]. Therefore, an InAs quantum dot creates a potential well for electrons in the  $n$ -GaAs matrix and for holes in  $p$ -GaAs one (Fig. 1). These potential wells can accumulate either a negative or a positive charge.

When the material of the InAs quantum dot is subjected to the non-uniform compressive deformation and the material of the GaAs matrix that surrounds the QD to the non-uniform tensile deformation, the band structure of the nanoheterosystem with QDs changes locally (Fig. 1,b). Owing to the self-consistent electron-deformation coupling, such a variation gives rise to a redistribution of the electron concentration in the vicinity of the stressed interface QD–matrix. As a result, there emerges an excess of negative charge in the material of the QD near the heterointerface, and its deficiency in the matrix material. Hence, there appears an  $n^+ - n$  junction (an electron-deformation dipole  $\mathbf{P}_{\text{el.}-\text{def}}$ ) at the stressed heterointerface QD–matrix.

**3. Calculation of the coordinate dependences of electrostatic potential and electron concentration in a spherical InAs quantum dot and the GaAs matrix**

The mathematical model of  $n^+ - n$  junction formation at a stressed heterointerface QD–matrix is described by the following self-consistent system of equations. First, it is the Schrödinger equation

$$\left[ \frac{\hbar^2}{2m_i^*} \Delta_{\mathbf{r}} + V_{\text{def}}^{(i)}(\mathbf{r}) - e\varphi_i(\mathbf{r}) \right] \psi_n^{(i)}(\mathbf{r}) = \tilde{E}_n \psi_n^{(i)}(\mathbf{r}),$$

$$i = \begin{cases} 1 \equiv \text{InAs} \\ 2 \equiv \text{GaAs} \end{cases}, \tag{1}$$

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

where  $\Delta E_c$  is the depth of the potential well for electrons in the InAs quantum dot in undeformed InAs/GaAs heterostructure,  $\tilde{E}_n = E_n - \lambda_0$  are the eigenvalues of the Schrödinger operator,  $\lambda_0$  is the bottom energy of non-deformed allowed band, and  $a_c^{(i)}$  is the constant of the hydrostatic deformation potential of the conduction band in the  $i$ -th material, and  $\varepsilon_i(\mathbf{r}) = \text{Sp } \hat{\varepsilon}_i$  is

the deformation parameter of the  $i$ -th material in the nanoheterostructure, which is determined by the atomic displacements  $\mathbf{u}_i$ . The latter are found from the equation of equilibrium

$$\nabla \operatorname{div} \mathbf{u}_i = -D^{(i)} \mathbf{F}^{(i)}(\mathbf{r}), \quad (3)$$

where  $\mathbf{F}^{(i)}(\mathbf{r}) = -e\delta\mathbf{E}^{(i)}$  and  $D^{(i)} = \frac{(1+\nu_i)(1-2\nu_i)}{a_{(i)}^3 E_i (1-\nu_i)}$ . Here,  $\delta\mathbf{E}$  is the excess electric field that emerges in the vicinity of the QD–matrix stressed interface, and its strength is determined as a gradient of the electrostatic potential  $\left(\delta E^{(i)} = -\frac{d\varphi^{(i)}(\mathbf{r})}{dr}\right)$ ,  $a_{(i)}$  is the lattice parameter of the  $i$ -th nanoheterostructure material,  $\nu_i$  is Poisson's ratio,  $E_i$  is the Young modulus, and  $e$  is the electron charge.

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

$$\Delta\varphi_i(\mathbf{r}) = \frac{e}{\varepsilon_d^{(i)} \varepsilon_0} \Delta n_i(\mathbf{r}), \quad (4)$$

where  $\varepsilon_d^{(i)}$  is the relative dielectric permittivity of the  $i$ -th nanoheterostructure material,  $\Delta n_i(\mathbf{r})$  is a variation of the electron concentration in the vicinity of the heterointerface QD–matrix. The electron concentration  $n_i(\mathbf{r})$  is determined in terms of a superposition of wave function products as

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

where the wave functions are the solutions of Schrödinger equation (1), and  $\mu_i$  is the chemical potential of the  $i$ -th nanoheterostructure material.

The system also includes an equation for the determination of chemical potential,

$$\frac{1}{\Omega_0} \int n(\mathbf{r}) d\mathbf{r} = n_0, \quad (6)$$

where  $\Omega_0$  is the elementary cell volume, and  $n_0$  is the average concentration of conduction electrons in the nanoheterostructure with QDs.

Since we consider a spherically symmetric nanoheterosystem (matrix + QD), which is justified for crystals with cubic symmetry, the system of equations (1)–(6) looks like

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

where  $R_{nl}^{(i)}(r)$  is the radial wave functions of electrons in the  $i$ -th semiconducting material. These functions are determined from the radial Schrödinger equation with deformation potential (2):

$$R_{nl}^{(1)}(r) = A j_l(k_{nl}r) + B n_l(k_{nl}r), \quad 0 \leq r \leq R_0,$$

$$R_{nl}^{(2)}(r) = C h_l^{(1)}(i\chi_{nl}r) + D h_l^{(2)}(i\chi_{nl}r), \quad R_0 \leq r \leq R_1, \quad (8)$$

where

$$k_{nl}^2 = \frac{2m_1^*}{\hbar^2} \left( |V_{\text{def}}^{(1)}| - |E_{nl}| \right),$$

$$\chi_{nl}^2 = \frac{2m_2^*}{\hbar^2} |E_{nl}|. \quad (9)$$

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

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

the regularity conditions for the functions  $R_{nl}^{(i)}(r)$  at  $r \rightarrow 0$  and  $r \rightarrow R_1$ , and the normalization conditions determine the energy spectrum  $E_{nl}$  and the wave functions of an electron in the InAs/GaAs heterosystem with an InAs quantum dot. The energy of the ground state of the electron in the QD is determined by the following transcendental equation:

$$k \operatorname{tg} \left( kR_0 - n\frac{\pi}{2} \right) = \chi \frac{m_1^*}{m_2^*} \frac{1 + \exp[2\chi(R_0 - R_1)]}{1 - \exp[2\chi(R_0 - R_1)]} + \\ + \frac{m_1^* - m_2^*}{R_0 m_2^*}, \quad n = 1. \quad (11)$$

The equation of equilibrium (3) looks like

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

where  $u_r^{(i)}$  is the radial component of an atomic displacement in the  $i$ -th semiconducting material. The general solution of the inhomogeneous equation (12) is tried as a sum

$$u_r^{(i)}(r) = u_{r \text{ mech}}^{(i)}(r) + u_{r \text{ el-def}}^{(i)}(r), \quad (13)$$

of the mechanical,  $u_{r\text{mech}}^{(i)}(r) = C_1^{(i)}r + \frac{C_2^{(i)}}{r^2}$ , and the electron-deformation,  $u_{r\text{el-def}}^{(i)}(r) = -\frac{D^{(i)}e}{r^2} \int r^2 \varphi^{(i)}(r) dr$ , displacement components.

For small concentrations of conduction electrons in the nanoheterosystem matrix ( $n_0 < 10^{18} \text{cm}^{-3}$ ), the values of the electron-deformation component of a displacement  $u_{r\text{el-def}}^{(i)}(r)$  at a QD are one order less than the mechanical component of a displacement  $u_{r\text{mech}}^{(i)}(r)$ . Therefore, we neglect the latter in the first approximation.

The displacement field determines the following components of the deformation tensor:

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

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

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

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

$$\begin{cases} u_r^{(2)}|_{r=R_0} - u_r^{(1)}|_{r=R_0} = f R_0, \\ \sigma_{rr}^{(1)}|_{r=R_0} = \sigma_{rr}^{(2)}|_{r=R_0} + P_L|_{r=R_0}, \quad P_L = \frac{2\alpha}{R_0 - |u_r^{(1)}|}, \\ \sigma_{rr}^{(2)}|_{r=R_1} = -\sigma_{ef}(N-1); \end{cases} \quad (17)$$

where  $\alpha$  is the surface energy of QD (InAs) [14],  $f = \frac{\alpha^{(1)} - \alpha^{(2)}}{\alpha^{(1)}} \approx 7\%$  is the parameter of a lattice mismatch between the contacting materials, and  $\sigma_{rr}^{(i)}$  is the radial component of the mechanical stress tensor for the  $i$ -th material [15].

We write the Poisson equation (4) as

$$\frac{d^2 \varphi^{(i)}}{dr^2} + \frac{2}{r} \frac{d\varphi^{(i)}}{dr} = \frac{e}{\varepsilon_d^{(i)} \varepsilon_0} (n_i(r) - n_0). \quad (18)$$

The concentration of charge carriers in the stressed nanoheterostructure with a QD was calculated adopting the model of  $\delta$ -like density of electron states in the QD:

$$\delta(E' - E_n) \approx \frac{1}{\sqrt{\pi/2} \Delta E} \exp\left(\frac{-2(E' - E_n)^2}{\Delta E^2}\right).$$

In particular, at the temperature  $T = 0$ , the distribution of charge carrier concentration  $n_i(r)$  in the QD

( $0 \leq r \leq R_0$ ) and the matrix ( $R_0 \leq r \leq R_1$ ) is determined by the formula

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

where  $N_{QD}$  is the surface concentration of QDs (for the InAs/GaAs nanoheterostructure with InAs quantum dots,  $N_{QD} \approx 3 \times 10^{10}$  [16]),  $\Delta E$  is the Gaussian curve half-width,  $E_1$  is the electron energy at the first localized level in the quantum well,  $\psi_{nlm}^{(i)}(r, \theta, \varphi) = R_{nl}^{(i)}(r) Y_{lm}(\theta, \varphi)$  is the solution of Schrödinger equation (1) in the spherical coordinate system, and  $Y_{lm}(\theta, \varphi)$  are the Legendre spherical functions [17].

Since the concentration of charge carriers  $n_i(r)$  in Poisson equation (18) is a nonlinear function of  $\varphi_i(r)$  [see Eq. (19)], we linearized it. Instead of expression (19), we used its expansion into Taylor's series:

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

The solution of Poisson equation (18) in the QD and the matrix, which took expression (20) for the electron concentration into account, was found for the averaged probability density  $|\bar{\psi}|^2$ . It looks like

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

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

where

$$Ei(z) = - \int_{-z}^{\infty} \frac{\exp(-t)}{t} dt,$$

$$\frac{1}{a_1} = \frac{e^2}{\varepsilon_d^{(1)} \varepsilon_0 a_{(1)}} |\bar{\psi}_1|^2 N_{\text{QD}} \frac{\sqrt{\frac{8}{\pi}}}{\Delta E} \times$$

$$\times \exp \left( \frac{-2 \left( \mu - E_1 - \lambda_0^{(1)} - a_c^{(1)} C_1^{(1)} \right)^2}{\Delta E^2} \right),$$

$$\frac{1}{a_2} = \frac{e^2}{\varepsilon_d^{(2)} \varepsilon_0 a_{(2)}} |\bar{\psi}_2|^2 N_{\text{QD}} \frac{\sqrt{\frac{8}{\pi}}}{\Delta E} \times$$

$$\times \exp \left( \frac{-2 \left( \mu - E_1 - \lambda_0^{(2)} - a_c^{(2)} C_1^{(2)} \right)^2}{\Delta E^2} \right),$$

$$d_2 = \frac{2a_c^{(2)} C_2^{(2)} e}{\varepsilon_d^{(2)} \varepsilon_0 a_{(2)}} |\bar{\psi}_2|^2 N_{\text{QD}} \frac{\sqrt{\frac{8}{\pi}}}{\Delta E} \times$$

$$\times \exp \left( \frac{-2 \left( \mu - E_1 - \lambda_0^{(2)} - a_c^{(2)} C_1^{(2)} \right)^2}{\Delta E^2} \right),$$

$$b_1 = \frac{e}{\varepsilon_d^{(1)} \varepsilon_0 a_{(1)}} |\bar{\psi}_1|^2 N_{\text{QD}} \left[ \operatorname{erf} \left( \frac{\sqrt{2}}{\Delta E} E_1 \right) + \right.$$

$$\left. + \operatorname{erf} \left( \frac{\sqrt{2}}{\Delta E} \left( \mu - E_1 - \lambda_0^{(1)} - a_c^{(1)} C_1^{(1)} \right) \right) - \frac{a^{(1)} n_0}{|\bar{\psi}_1|^2 N_{\text{QD}}} \right],$$

$$b_2 = \frac{e}{\varepsilon_d^{(2)} \varepsilon_0 a_{(2)}} |\bar{\psi}_2|^2 N_{\text{QD}} \left[ \operatorname{erf} \left( \frac{\sqrt{2}}{\Delta E} E_1 \right) + \right.$$

$$\left. + \operatorname{erf} \left( \frac{\sqrt{2}}{\Delta E} \left( \mu - E_1 - \lambda_0^{(2)} - a_c^{(2)} C_1^{(2)} \right) \right) - \frac{a^{(2)} n_0}{|\bar{\psi}_2|^2 N_{\text{QD}}} \right].$$

The coefficients  $A_1$ ,  $B_1$ , and  $B_2$  in expressions (21) and (22) are determined using the continuity conditions for the potentials  $\varphi_1(r)$  and  $\varphi_2(r)$  and the normal component of the electric displacement vector at the stressed heterointerface and the electroneutrality condition

$$\begin{cases} \varphi^{(1)}(r)|_{r=R_0} = \varphi^{(2)}(r)|_{r=R_0} \\ \varepsilon_1 \frac{d\varphi^{(1)}(r)}{dr} \Big|_{r=R_0} = \varepsilon_2 \frac{d\varphi^{(2)}(r)}{dr} \Big|_{r=R_0} \\ \int_0^{R_0} r^2 \Delta n_1(r) dr + \int_{R_0}^{R_1} r^2 \Delta n_2(r) dr = 0. \end{cases} \quad (23)$$

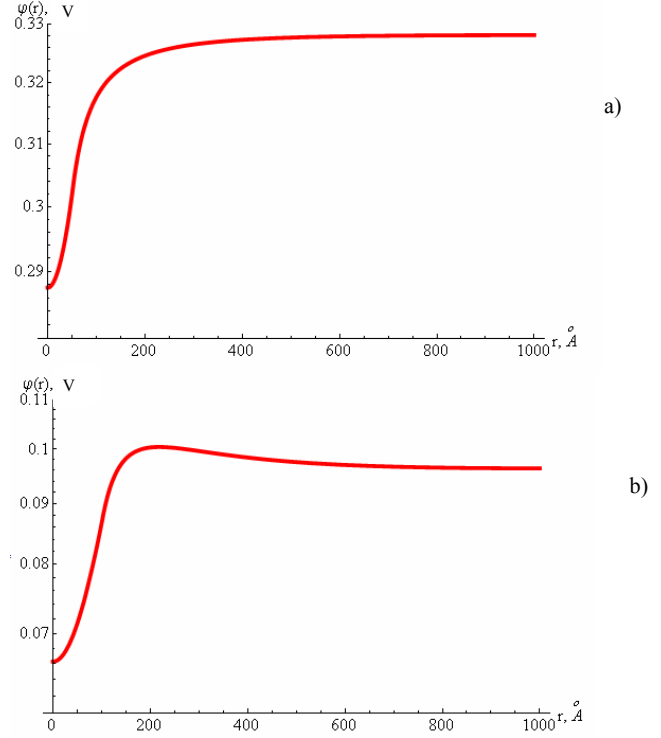


Fig. 2. Coordinate dependences of the electrostatic potential  $\varphi(r)$  in the nanoheterosystem with QDs with dimensions  $R_0 = 50$  (a) and  $100 \text{ \AA}$  (b)

#### 4. Numerical Calculations and Discussion of the Results Obtained

In this section, we present the numerical results of theoretical researches of the coordinate dependences of the electrostatic potential and the electron concentration in the QD and the matrix for the InAs/GaAs nanoheterosystem obtained in the framework of the deformation potential model. The system parameters are as follows [14, 18, 19]:  $a^{(1)} = 6.08 \text{ \AA}$ ,  $a^{(2)} = 5.65 \text{ \AA}$ ,  $C_{11}^{(1)} = 0.833 \text{ Mbar}$ ,  $C_{12}^{(1)} = 0.453 \text{ Mbar}$ ,  $C_{11}^{(2)} = 1.223 \text{ Mbar}$ ,  $C_{12}^{(2)} = 0.571 \text{ Mbar}$ ,  $\Delta E_c(0) = 830 \text{ meV}$ ,  $a_c^{(1)} = -5.08 \text{ eV}$ ,  $a_c^{(2)} = -7.17 \text{ eV}$ ,  $E_g^{(1)}(0) = 0.36 \text{ eV}$ ,  $E_g^{(2)}(0) = 1.452 \text{ eV}$ ,  $R_1 = 1000 \text{ \AA}$ ;  $\sigma_{\text{eff}} = 10^9 \text{ N/m}^2$ ,  $m_1^{(e)} = 0.057m_0$ ,  $m_2^{(e)} = 0.065m_0$ , and  $\alpha = 0.657 \text{ N/m}$ .

In Figs. 2 and 3, the coordinate dependences of the electrostatic potential  $\varphi(r)$  and the redistribution of electron concentration  $\Delta n(r)$ , respectively, in the InAs/GaAs nanoheterosystem including InAs quantum dots with dimensions  $R_0 = 50$  and  $100 \text{ \AA}$  are depicted.

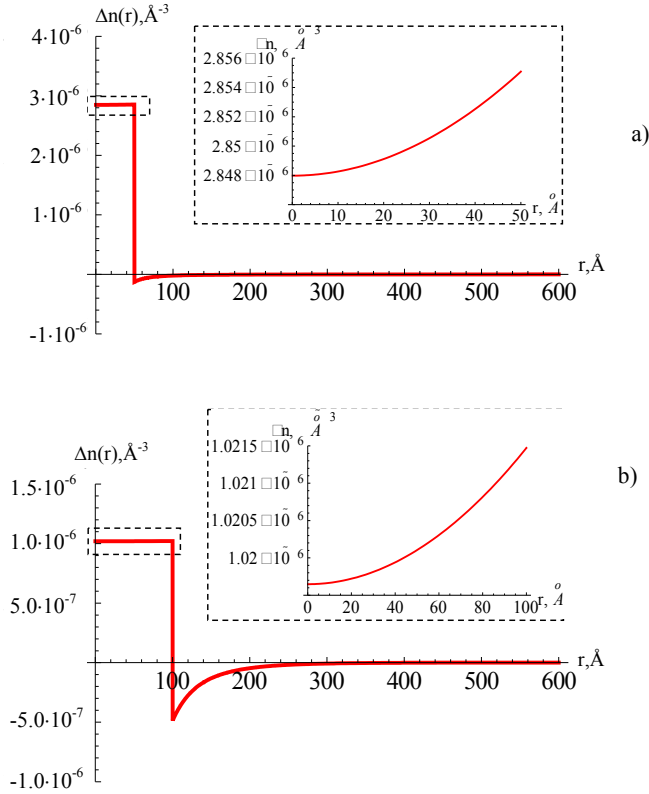


Fig. 3. Coordinate dependences of the electron concentration  $\Delta n(r)$  in the nanoheterosystem with QDs with dimensions  $R_0 = 50$  (a) and  $100 \text{ \AA}$  (b)

One can see (Fig. 2) that the potential  $\varphi(r)$  in this nanoheterosystem falls down, if the QD size grows. In particular, the increase of the QD radius from  $50$  to  $100 \text{ \AA}$  brings about a reduction of the electrostatic potential at the interface QD–matrix by approximately  $206 \text{ meV}$ .

Depending on the QD dimensions, the potential distribution  $\varphi(r)$  in such a nanoheterosystem has either a monotonous (Fig. 2,a) or a nonmonotonous (Fig. 2,b) character. In particular, for QDs with  $R_0 = 20 \div 70 \text{ \AA}$ , the coordinate dependence of electrostatic potential is monotonous, whereas, if  $R_0 > 70 \text{ \AA}$ , it is nonmonotonous and has a maximum, whose position is determined by the QD radius. Such a character of the electrostatic potential distribution  $\varphi(r)$  in QDs with different dimensions is governed by the redistribution of the electron concentration  $\Delta n = \Delta n(\mathbf{r})$  (Fig. 3) in the vicinity of the QD–matrix interface. In the QD itself, the potential  $\varphi(r)$  varies strongly, but when the distance from the QD–matrix interface grows ( $r \rightarrow R_1$ ), it tends to the value  $\varphi(r)|_{r=R_1} \approx (B_2/R_1) \exp(R_1/\sqrt{a_2}) - a_2 b_2$ .

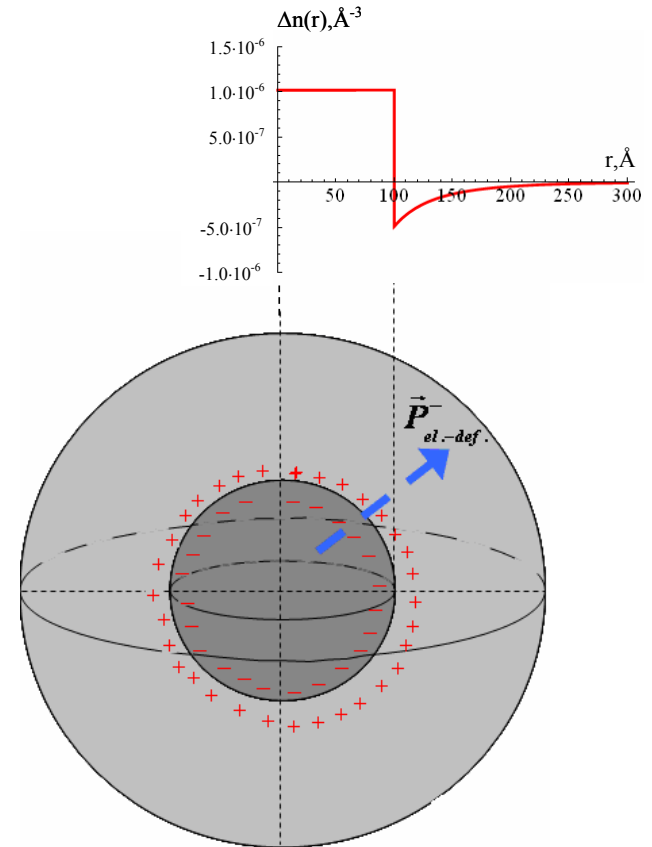


Fig. 4. Geometrical representation of the  $n^+ - n$  junction at the QD–matrix interface

The plots presented in Fig. 3 clearly demonstrate that, in the vicinity of the QD–matrix interface, there occurs a spatial redistribution of electrons, so that there emerge an excess of electrons in the QD near the interface and an electron deficiency in the matrix. Electrostatic interaction between charges leads to such a redistribution of the electron concentration that there arises an electric double layer, i.e. an  $n^+ - n$  junction, at the QD–matrix interface (Fig. 4). The profile of the majority charge carrier concentration in the vicinity of the QD–matrix interface can be determined from experimental C–V characteristics, by using the formula [20]

$$n^{(i)}(r_W) = 2 \left[ \varepsilon_d^{(i)} \varepsilon_0 A^2 \frac{d}{dV} \left( \frac{1}{C^2} \right) \right]^{-1},$$

where  $A$  is the area of the contact between the QD and the matrix, and  $r_W$  is the running coordinate of the space charge region boundary. The electric properties of the  $n^+ - n$  junction can be controlled technologically by varying the surface concentration of quantum dots,  $N_{QD}$ .

A reduction of the QD symmetry will not result in the disappearance of  $p - n$  ( $n^+ - n, p^+ - p$ ) junctions at the QD–matrix interface. It only will induce the anisotropy of electric properties of those junctions.

The presence of  $p - n$  ( $n^+ - n, p^+ - p$ ) junctions at the QD–matrix interface can be detected by measuring the current-voltage characteristic (CVC) of the nanocontact between the QD and the matrix [9, 21].

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#### ФОРМУВАННЯ $n^+ - n$ ПЕРЕХОДІВ НА НАПРУЖЕНІЙ МЕЖІ КВАНТОВА ТОЧКА–МАТРИЦЯ

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#### Резюме

В межах моделі самоузгодженого електрон-деформаційного зв'язку побудовано теорію формування  $n^+ - n$  переходів у напружених наногетеросистемах з квантовими точками. Показано, що на напруженій межі квантова точка – матриця виникає подвійний електричний шар, тобто  $n^+ - n$  перехід.