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On Approach for Prognosis of Influence of Mismatch-induced Stresses on the I–V Characteristics of p-n-junctions Manufactured in a Heterostructure

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Abstract: We consider a nonlinear model for analysis of current-voltage characteristic of a *p*-*n*-junction, which was manufactured in the framework of a heterostructure with specific configuration by diffusion or ion implantation. We analyzed the model to obtain dependence of the considered current-voltage characteristic on missmatch-induced stresses in the framework of the heterostructure. We also consider an analytical approach for analysis of mass and heat transport during the considered processes with account their nonlinearity and missmatch induced stresses as well changes of parameters of these in space and time.
Keywords: *p*-*n*-junctions; Current-voltage characteristics; Influence of missmatch-induced stresses; Analytical approach for prognosis.

1. Introduction

Manufacturing of new microelectronic devices and improvement of existing ones are the basis for manufacturing of new integrated circuits [1-5]. Both during manufacturing of new types of microelectronic devices and for improvement of existing ones, it is necessary to analyze the processes that occur both during the manufacturing of devices and during their operation [1-5]. In this paper we consider a two-layer structure, which consist of a substrate and an epitaxial layer (see Figs. 1 and 2). A dopant has been infused or implanted in the epitaxial layer. The infusion and implantation generate necessary type of conductivity (*p* or *n*) in the epitaxial layer. Under special conditions for annealing, sharpness of the *p*-*n*-junction increases. The increasing leads to changes of charge carriers transport [6-9]. The transport of charge carriers could be also changes under influence of missmatch induced stress in heterostructures. The main aim of this work is analysis of influence of missmatch induced stress on the charge carriers transport. The accompanying aim of this paper is the choosing of a mathematical apparatus for the analysis of the considered transport.

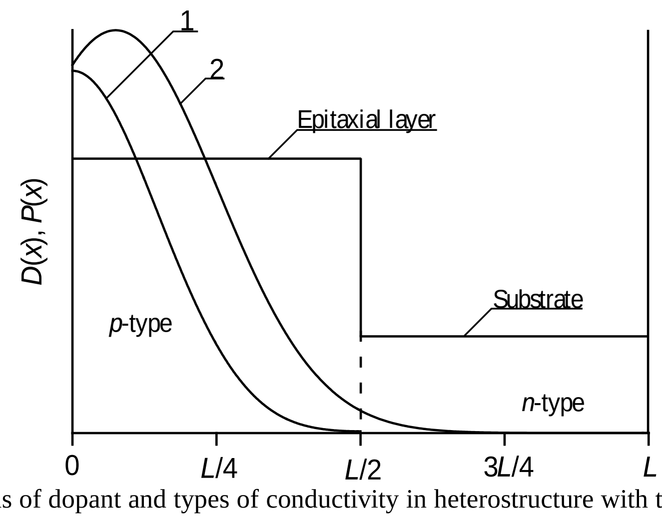

Fig. 1. Initial distributions of dopant and types of conductivity in heterostructure with two layers. Curves 1 and 2 are the typical distributions of concentration of dopand (for diffusion and ion types of doping)

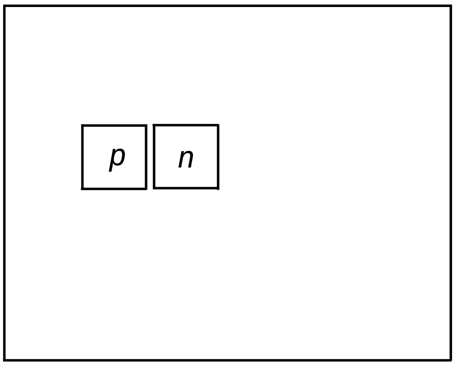

Fig. 2. View from top on area of *p-n*-junction, manufactured in considered epitaxial layer

The qualitative structure of the *p-n*-junction is shown in Fig. 3. In this figure and further in the text, the following notations were introduced: φ_k is the contact potential difference; $U(t)$ is the applied voltage; L_n and $-L_p$ are the boundaries of the *p-n*- junction region.

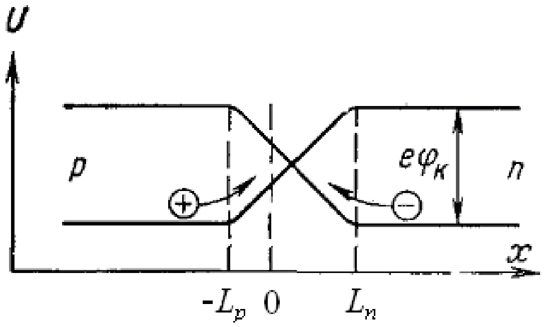

Fig. 3. Qualitative structure of the *p-n*- junction.

2. Method of solution

We describe spatio-temporal distributions of charge carriers in *p-n*-junction area as a solution of following system of equations [1,10,11]

$$\frac{\partial n(x,y,z,t)}{\partial t}=G+\frac{\partial}{\partial x}\left[D_n\frac{\partial n(x,y,z,t)}{\partial x}\right]+\frac{\partial}{\partial y}\left[D_n\frac{\partial n(x,y,z,t)}{\partial y}\right]+\frac{\partial}{\partial z}\left[D_n\frac{\partial n(x,y,z,t)}{\partial z}\right]-k_{np}\left[n(x,y,z,t)\times\right.$$
$$\left.\times p(x,y,z,t)-n_0p_0\right]+\Omega\frac{\partial}{\partial x}\left[\frac{D_{Sn}}{kT}\nabla_S\mu_h(x,y,z,t)\int_0^{L_z}n(x,y,W,t)\,dW\right]+\Omega\frac{\partial}{\partial y}\left[\frac{D_{Sn}}{kT}\nabla_S\mu_h(x,y,z,t)\int_0^{L_z}n(x,y,W,t)\,dW\right]-$$
$$-\frac{\partial}{\partial x}\left\{\mu_n n(x,y,z,t)\frac{\partial\left[\varphi(x,y,z,t)+\varphi_h(x,y,z,t)\right]}{\partial x}\right\}-\frac{\partial}{\partial y}\left\{\mu_n n(x,y,z,t)\frac{\partial\left[\varphi(x,y,z,t)+\varphi_h(x,y,z,t)\right]}{\partial y}\right\},\qquad(1)$$
$$\frac{\partial p(x,y,z,t)}{\partial t}=G+\frac{\partial}{\partial x}\left[D_p\frac{\partial p(x,y,z,t)}{\partial x}\right]+\frac{\partial}{\partial y}\left[D_p\frac{\partial p(x,y,z,t)}{\partial y}\right]+\frac{\partial}{\partial z}\left[D_p\frac{\partial n(x,y,z,t)}{\partial z}\right]-k_{np}\left[n(x,y,z,t)\times\right.$$
$$\left.\times p(x,y,z,t)-n_0p_0\right]+\Omega\frac{\partial}{\partial x}\left[\frac{D_{Sp}}{kT}\nabla_S\mu_h(x,y,z,t)\int_0^{L_z}p(x,y,W,t)\,dW\right]+\Omega\frac{\partial}{\partial y}\left[\frac{D_{Sp}}{kT}\nabla_S\mu_h(x,y,z,t)\int_0^{L_z}p(x,y,W,t)\,dW\right]-$$
$$-\frac{\partial}{\partial x}\left\{\mu_n p(x,y,z,t)\frac{\partial\left[\varphi(x,y,z,t)+\varphi_h(x,y,z,t)\right]}{\partial x}\right\}-\frac{\partial}{\partial y}\left\{\mu_n p(x,y,z,t)\frac{\partial\left[\varphi(x,y,z,t)+\varphi_h(x,y,z,t)\right]}{\partial y}\right\},$$

where $\rho(x,y,z,t)$ ($\rho = n, p$) are the spatio-temporal (x, y and z are the coordinate, t is the time) distributions of concentrations of electrons (for $\rho = n$) and holes (for $\rho = p$); ρ_0 is the equilibrium distributions of charge carriers; D_ρ and $D_{\rho S}$ are the coefficients of volumetric and surficial diffusions (due to miss-match induced stress); μ_ρ is the charge carriers mobility; $\int_0^{L_z}\rho(x,y,z,t)dz$ is the surficial concentration of charge carriers on the interface between layers of the considered heterostructure (we assume, that axis Oz is perpendicular to interface between layers of the considered heterostructure); $\mu_h(x,y,z,t)$ is the chemical potential due to miss-match induced stress; $\varphi(x,y,z,t)$ is the distribution of electrical potential in area of space charge; $\varphi_h(x,y,z,t)$ is the potential barrier of the heterojunction; G is the speed of generation of electron-hole pares; k_{np} is the parameter of recombination. Boundary and initial conditions for the Eqs. (1) could be written as

$$n(L_n,y,z,t) = n_n(z,t),\ n(-L_p,y,z,t) = n_p(x,y,z,t),\ p(L_n,y,z,t) = p_n(x,y,z,t),\ p(-L_p,y,z,t) = p_p(x,y,z,t),\ n(x,L_n,z,t) = n_n(x,y,z,t),$$
$$n(x,-L_p,z,t) = n_p(x,y,z,t),\ p(x,L_n,z,t) = p_n(x,y,z,t),\ p(x,-L_p,z,t) = p_p(x,y,z,t),\ n(x,y,L_n,t) = n_n(x,y,L_n,t),\ n(x,y,-L_p,t) = n_p(x,y,-L_p,t),$$
$$p(x,y,L_n,t) = p_n(x,y,L_n,t),\ p(x,y,-L_p,t) = p_p(x,y,-L_p,t),\ n(x,y,z,0) = n_0(x,y,z),\ p(x,y,z,0) = p_0(x,y,z). \tag{2}$$

We calculate distribution of potential in space charge area by solution of Poisson equation in the following form

$$\frac{\partial^2\varphi(x,y,z,t)}{\partial x^2}+\frac{\partial^2\varphi(x,y,z,t)}{\partial y^2}+\frac{\partial^2\varphi(x,y,z,t)}{\partial z^2}=e\frac{N_a(x,y,z,t)-N_d(x,y,z,t)}{\varepsilon\,\varepsilon_0}, \tag{3}$$

where $N_a(x,y,z,t)$ and $N_d(x,y,z,t)$ are the spatio-temporal distributions of acceptor and donor impurity; e is the elementary charge; ε is the dielectric constant of materials; $\varepsilon_0 \approx 8{,}85\cdot10^{-12}$ F/m is the dielectric constant. Boundary and initial conditions for the Poisson equation takes the form

$$\varphi(L_n,y,z,t) = \varphi_k+U(t),\ \varphi(-L_p,y,z,t) = U(t),\ \varphi(x,L_n,z,t) \approx 0,\ \varphi(x,-L_p,z,t) \approx 0,\ \varphi(x,y,L_n,t) \approx 0,\ \varphi(x,y,-L_p,t) \approx \varphi_h, \tag{4}$$

where $U(t)$ is the applied difference of potentials. Further we will consider case of single ionization, when $N_a(x,y,z,t) = p(x,y,z,t)$ and $N_d(x,y,z,t) = n(x,y,z,t)$. Then

$$\frac{\partial^2\varphi(x,y,z,t)}{\partial x^2}+\frac{\partial^2\varphi(x,y,z,t)}{\partial y^2}+\frac{\partial^2\varphi(x,y,z,t)}{\partial z^2}=e\frac{p(x,y,z,t)-n(x,y,z,t)}{\varepsilon\,\varepsilon_0}. \tag{5}$$

Solution of the Eq. (5) is the following function

$$\varphi(x,y,z,t)=\left\{\varphi_k+U(t)-\frac{e}{\varepsilon\,\varepsilon_0}\int\limits_{-L_p}^{L_n}(L_n-u)\int\limits_{-L_p}^{L_n}(L_n-v)\int\limits_{-L_p}^{L_n}(L_n-w)[p(u,v,w,t)-n(u,v,w,t)]\,d\,w\,d\,v\,d\,u\right\}\frac{x-L_n}{L_p+L_n}\frac{y-L_n}{L_p+L_n}\times$$
$$\times\frac{z-L_n}{L_p+L_n}+\varphi_h+\varphi_k+U(t)-\frac{e}{\varepsilon\,\varepsilon_0}\int\limits_{x}^{L_n}(L_n-u)\int\limits_{y}^{L_n}(L_n-v)\int\limits_{z}^{L_n}[p(u,v,w,t)-n(u,v,w,t)]\,d\,w\,d\,v\,d\,u\,. \tag{6}$$

Chemical potential μ_h in Eqs. (1) could be determine by using the following relation [15]

$$\mu_h=E(z)\Omega\sigma_{ij}\,[u_{ij}(x,y,z,t)+u_{ji}(x,y,z,t)]/2, \tag{7}$$

where E is the tensile modulus (Young); σ_{ij} is the stress tensor; $u_{ij}=\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)$ is the deformation tensor; u_i, u_j are the components $u_x(x,y,z,t)$, $u_y(x,y,z,t)$ and $u_z(x,y,z,t)$ displacement vector $\vec{u}(x,y,z,t)$; x_i, x_j are the coordinates x, y, z. Relation (7) could be transformed to the following form

$$\mu_h(x,y,z,t)=E(z)\frac{\Omega}{2}\left[\frac{\partial u_i(x,y,z,t)}{\partial x_j}+\frac{\partial u_j(x,y,z,t)}{\partial x_i}\right]\left\{\frac{1}{2}\left[\frac{\partial u_i(x,y,z,t)}{\partial x_j}+\frac{\partial u_j(x,y,z,t)}{\partial x_i}\right]+\left[\frac{\partial u_k(x,y,z,t)}{\partial x_k}-3\varepsilon_0\right]\times\right.$$
$$\left.\times\frac{\sigma(z)\delta_{ij}}{1-2\sigma(z)}-\varepsilon_0\delta_{ij}-K(z)\beta(z)\,[T(x,y,z,t)-T_0]\,\delta_{ij}\right\},$$

where σ is the Poisson coefficient; $\varepsilon_0=(a_s-a_{EL})/a_{EL}$ is the lattice mismatch parameter; a_s, a_{EL} are the lattice constants of the substrate and the epitaxial layer; K is the compression module; β is the coefficient of thermal expansion; T_r

is the equilibrium temperature, which coincides with the room temperature. Components of displacement vector could be calculated by solution of the following system of equations [11]

$$\rho(z)\frac{\partial^2 u_x(x,y,z,t)}{\partial t^2}=\frac{\partial \sigma_{xx}(x,y,z,t)}{\partial x}+\frac{\partial \sigma_{xy}(x,y,z,t)}{\partial y}+\frac{\partial \sigma_{xz}(x,y,z,t)}{\partial z}$$

$$\rho(z)\frac{\partial^2 u_y(x,y,z,t)}{\partial t^2}=\frac{\partial \sigma_{yx}(x,y,z,t)}{\partial x}+\frac{\partial \sigma_{yy}(x,y,z,t)}{\partial y}+\frac{\partial \sigma_{yz}(x,y,z,t)}{\partial z}$$

$$\rho(z)\frac{\partial^2 u_z(x,y,z,t)}{\partial t^2}=\frac{\partial \sigma_{zx}(x,y,z,t)}{\partial x}+\frac{\partial \sigma_{zy}(x,y,z,t)}{\partial y}+\frac{\partial \sigma_{zz}(x,y,z,t)}{\partial z}$$

where

$$\sigma_{ij}=\frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial u_i(x,y,z,t)}{\partial x_j}+\frac{\partial u_j(x,y,z,t)}{\partial x_i}-\frac{\delta_{ij}}{3}\frac{\partial u_k(x,y,z,t)}{\partial x_k}\right]+K(z)\delta_{ij}\frac{\partial u_k(x,y,z,t)}{\partial x_k}-\left[T(x,y,z,t)-T_r\right]\times$$
$$\times\,\beta(z)\,K(z),$$

$\rho(z)$ is the density of materials of heterostructures; δ_{ij} is the Kronecker symbol. Accounting of the above relation transforms the previous system of equations to the following form

$$\rho(z)\frac{\partial^2 u_x(x,y,z,t)}{\partial t^2}=\left\{K(z)+\frac{5E(z)}{6[1+\sigma(z)]}\right\}\frac{\partial^2 u_x(x,y,z,t)}{\partial x^2}+\left\{K(z)-\frac{E(z)}{3[1+\sigma(z)]}\right\}\frac{\partial^2 u_y(x,y,z,t)}{\partial x\partial y}+\frac{E(z)}{2[1+\sigma(z)]}\times$$
$$\times\left[\frac{\partial^2 u_y(x,y,z,t)}{\partial y^2}+\frac{\partial^2 u_z(x,y,z,t)}{\partial z^2}\right]+\left\{K(z)+\frac{E(z)}{3[1+\sigma(z)]}\right\}\frac{\partial^2 u_z(x,y,z,t)}{\partial x\partial z}-K(z)\beta(z)\frac{\partial T(x,y,z,t)}{\partial x}$$

$$\rho(z)\frac{\partial^2 u_y(x,y,z,t)}{\partial t^2}=\frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial^2 u_y(x,y,z,t)}{\partial x^2}+\frac{\partial^2 u_x(x,y,z,t)}{\partial x\partial y}\right]-K(z)\beta(z)\frac{\partial T(x,y,z,t)}{\partial y}+\frac{\partial^2 u_y(x,y,z,t)}{\partial y^2}\times$$
$$\times\left\{\frac{5E(z)}{12[1+\sigma(z)]}+K(z)\right\}+\left\{K(z)-\frac{E(z)}{6[1+\sigma(z)]}\right\}\frac{\partial^2 u_y(x,y,z,t)}{\partial y\partial z}+\frac{\partial}{\partial z}\left\{\frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial u_y(x,y,z,t)}{\partial z}+\frac{\partial u_z(x,y,z,t)}{\partial y}\right]\right\}+$$
$$+K(z)\frac{\partial^2 u_y(x,y,z,t)}{\partial x\partial y} \tag{8}$$

$$\rho(z)\frac{\partial^2 u_z(x,y,z,t)}{\partial t^2}=\frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial^2 u_z(x,y,z,t)}{\partial x^2}+\frac{\partial^2 u_z(x,y,z,t)}{\partial y^2}+\frac{\partial^2 u_x(x,y,z,t)}{\partial x\partial z}+\frac{\partial^2 u_y(x,y,z,t)}{\partial y\,\partial z}\right]+$$
$$+\left.\frac{\partial^2 u_y(x,y,z,t)}{\partial y\partial z}\right]+\frac{\partial}{\partial z}\left\{K(z)\left[\frac{\partial u_x(x,y,z,t)}{\partial x}+\frac{\partial u_y(x,y,z,t)}{\partial y}+\frac{\partial u_x(x,y,z,t)}{\partial z}\right]\right\}-K(z)\beta(z)\frac{\partial T(x,y,z,t)}{\partial z}+$$
$$+\frac{1}{6}\frac{\partial}{\partial z}\left\{\frac{E(z)}{1+\sigma(z)}\left[6\frac{\partial u_z(x,y,z,t)}{\partial z}-\frac{\partial u_x(x,y,z,t)}{\partial x}-\frac{\partial u_y(x,y,z,t)}{\partial y}-\frac{\partial u_z(x,y,z,t)}{\partial z}\right]\right\}.$$

System of conditions for these equations could be presented in the following form

$$\left.\frac{\partial\,\vec{u}(x,y,z,t)}{\partial x}\right|_{x=0}=0\,;\ \left.\frac{\partial\,\vec{u}(x,y,z,t)}{\partial x}\right|_{x=L_x}=0\,;\ \left.\frac{\partial\,\vec{u}(x,y,z,t)}{\partial y}\right|_{y=0}=0\,;\ \left.\frac{\partial\,\vec{u}(x,y,z,t)}{\partial y}\right|_{y=L_y}=0\,;$$
$$\left.\frac{\partial\,\vec{u}(x,y,z,t)}{\partial z}\right|_{z=0}=0\,;$$
$$\left.\frac{\partial\,\vec{u}(x,y,z,t)}{\partial z}\right|_{z=L_z}=0\,;\ \vec{u}(x,y,z,0)=\vec{u}_0\,;\ \vec{u}(x,y,z,\infty)=\vec{u}_0\,.$$

Farther we calculate components of displacement vector by solutions of equations of system (8). To calculate the first-order approximations of required components framework method of averaging of functional corrections we substitute their not yet known average values α_i into the right sides of Eqs. (8). The substitution leads to the following result

$$\rho(z)\frac{\partial^2 u_{1x}(x,y,z,t)}{\partial t^2} = -K(z)\beta(z)\frac{\partial T(x,y,z,t)}{\partial x},$$
$$\rho(z)\frac{\partial^2 u_{1y}(x,y,z,t)}{\partial t^2} = -K(z)\beta(z)\frac{\partial T(x,y,z,t)}{\partial y},$$
$$\rho(z)\frac{\partial^2 u_{1z}(x,y,z,t)}{\partial t^2} = -K(z)\beta(z)\frac{\partial T(x,y,z,t)}{\partial z}.$$

Integration of these equations on time t gives a possibility to obtain the first-order approximations of required components in the following form

$$u_{1x}(x,y,z,t) = K(z)\frac{\beta(z)}{\rho(z)}\frac{\partial}{\partial x}\int_0^t\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta - K(z)\frac{\beta(z)}{\rho(z)}\frac{\partial}{\partial x}\int_0^\infty\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta + u_{0x},$$
$$u_{1y}(x,y,z,t) = K(z)\frac{\beta(z)}{\rho(z)}\frac{\partial}{\partial y}\int_0^t\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta - K(z)\frac{\beta(z)}{\rho(z)}\frac{\partial}{\partial y}\int_0^\infty\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta + u_{0y},$$
$$u_{1z}(x,y,z,t) = K(z)\frac{\beta(z)}{\rho(z)}\frac{\partial}{\partial z}\int_0^t\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta - K(z)\frac{\beta(z)}{\rho(z)}\frac{\partial}{\partial z}\int_0^\infty\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta + u_{0z}.$$

Approximations with the second and higher orders of components of displacement vector could be calculated by using standard replacement of required functions in right sides of Eqs. (8) on the following sum $\alpha_i+u_i(x,y,z,t)$ [12]. The replacement leads to the following result

$$\rho(z)\frac{\partial^2 u_{2x}(x,y,z,t)}{\partial t^2} = \left\{K(z)+\frac{5E(z)}{6[1+\sigma(z)]}\right\}\frac{\partial^2 u_{1x}(x,y,z,t)}{\partial x^2} + \left\{K(z)-\frac{E(z)}{3[1+\sigma(z)]}\right\}\frac{\partial^2 u_{1y}(x,y,z,t)}{\partial x\,\partial y} + \frac{E(z)}{2[1+\sigma(z)]}\times$$
$$\times\left[\frac{\partial^2 u_{1y}(x,y,z,t)}{\partial y^2} + \frac{\partial^2 u_{1z}(x,y,z,t)}{\partial z^2}\right] + \left\{K(z)+\frac{E(z)}{3[1+\sigma(z)]}\right\}\frac{\partial^2 u_{1z}(x,y,z,t)}{\partial x\,\partial z} - K(z)\beta(z)\frac{\partial T(x,y,z,t)}{\partial x}$$
$$\rho(z)\frac{\partial^2 u_{2y}(x,y,z,t)}{\partial t^2} = \frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial^2 u_{1y}(x,y,z,t)}{\partial x^2} + \frac{\partial^2 u_{1x}(x,y,z,t)}{\partial x\,\partial y}\right] - K(z)\beta(z)\frac{\partial T(x,y,z,t)}{\partial y} + K(z)\frac{\partial^2 u_{1y}(x,y,z,t)}{\partial x\,\partial y} +$$
$$+\frac{\partial}{\partial z}\left\{\frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial u_{1y}(x,y,z,t)}{\partial z} + \frac{\partial u_{1z}(x,y,z,t)}{\partial y}\right]\right\} + \frac{\partial^2 u_{1y}(x,y,z,t)}{\partial y^2}\left\{\frac{5E(z)}{12[1+\sigma(z)]} + K(z)\right\} + \left\{K(z)-\frac{E(z)}{6[1+\sigma(z)]}\right\}\times$$
$$\times\frac{\partial^2 u_{1y}(x,y,z,t)}{\partial y\,\partial z}$$
$$\rho(z)\frac{\partial^2 u_{2z}(x,y,z,t)}{\partial t^2} = \frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial^2 u_{1z}(x,y,z,t)}{\partial x^2} + \frac{\partial^2 u_{1z}(x,y,z,t)}{\partial y^2} + \frac{\partial^2 u_{1x}(x,y,z,t)}{\partial x\,\partial z} + \frac{\partial^2 u_{1y}(x,y,z,t)}{\partial y\,\partial z}\right] +$$
$$+\frac{\partial}{\partial z}\left\{K(z)\left[\frac{\partial u_{1x}(x,y,z,t)}{\partial x} + \frac{\partial u_{1y}(x,y,z,t)}{\partial y} + \frac{\partial u_{1x}(x,y,z,t)}{\partial z}\right]\right\} - K(z)\beta(z)\frac{\partial T(x,y,z,t)}{\partial z} +$$
$$+\frac{1}{6}\frac{\partial}{\partial z}\left\{\frac{E(z)}{1+\sigma(z)}\left[6\frac{\partial u_{1z}(x,y,z,t)}{\partial z} - \frac{\partial u_{1x}(x,y,z,t)}{\partial x} - \frac{\partial u_{1y}(x,y,z,t)}{\partial y} - \frac{\partial u_{1z}(x,y,z,t)}{\partial z}\right]\right\}.$$

Integration of right and left sides of obtained relations on time t leads to the following result

$$u_{2x}(x,y,z,t) = \frac{1}{\rho(z)}\left\{K(z)+\frac{5E(z)}{6[1+\sigma(z)]}\right\}\frac{\partial^2}{\partial x^2}\int_0^t\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta + \frac{1}{\rho(z)}\left\{K(z)-\frac{E(z)}{3[1+\sigma(z)]}\right\}\times$$
$$\times\frac{\partial^2}{\partial x\,\partial y}\int_0^t\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta + \frac{E(z)}{\rho(z)[1+\sigma(z)]}\left[\frac{\partial^2}{\partial y^2}\int_0^t\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta + \frac{\partial^2}{\partial z^2}\int_0^t\int_0^\vartheta u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta\right] +$$

$$+\frac{1}{\rho(z)}\left\{K(z)+\frac{E(z)}{3\,[1+\sigma(z)]}\right\}\frac{\partial^2}{\partial x\,\partial z}\int_0^t\int_0^\vartheta u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta-K(z)\frac{\beta(z)}{\rho(z)}\frac{\partial}{\partial x}\int_0^t\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta-\left\{K(z)+\frac{5\,E(z)}{6\,[1+\sigma(z)]}\right\}\times$$

$$\times\frac{1}{\rho(z)}\frac{\partial^2}{\partial x^2}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta-\frac{1}{\rho(z)}\left\{K(z)-\frac{E(z)}{3[1+\sigma(z)]}\right\}\frac{\partial^2}{\partial x\,\partial y}\int_0^\infty\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta-\frac{E(z)}{2\,\rho(z)[1+\sigma(z)]}\times$$

$$\times\left[\frac{\partial^2}{\partial y^2}\int_0^\infty\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{\partial^2}{\partial z^2}\int_0^\infty\int_0^\vartheta u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta\right]-\left\{K(z)+\frac{E(z)}{3\,[1+\sigma(z)]}\right\}\frac{\partial^2}{\partial x\,\partial z}\int_0^\infty\int_0^\vartheta u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta\,\times$$

$$\times\frac{1}{\rho(z)}+K(z)\frac{\beta(z)}{\rho(z)}\frac{\partial}{\partial x}\int_0^\infty\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta+u_{0x}$$

$$u_{2y}(x,y,z,t)=\frac{E(z)}{2\,\rho(z)[1+\sigma(z)]}\left[\frac{\partial^2}{\partial x^2}\int_0^t\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{\partial^2}{\partial x\,\partial y}\int_0^t\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta\right]+\frac{K(z)}{\rho(z)}\times$$

$$\times\frac{\partial^2}{\partial x\,\partial y}\int_0^t\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{1}{\rho(z)}\frac{\partial^2}{\partial y^2}\int_0^t\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta\left\{\frac{5E(z)}{12\,[1+\sigma(z)]}+K(z)\right\}+\frac{1}{2\rho(z)}\frac{\partial}{\partial z}\left\{\frac{E(z)}{1+\sigma(z)}\times\right.$$

$$\left.\times\left[\frac{\partial}{\partial z}\int_0^t\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{\partial}{\partial y}\int_0^t\int_0^\vartheta u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta\right]\right\}-K(z)\frac{\beta(z)}{\rho(z)}\int_0^t\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{1}{\rho(z)}\left\{K(z)-\right.$$

$$\left.-\frac{E(z)}{6[1+\sigma(z)]}\right\}\int_0^t\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{1}{\rho(z)}\left\{K(z)-\frac{E(z)}{6[1+\sigma(z)]}\right\}\frac{\partial^2}{\partial y\,\partial z}\int_0^t\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta-\frac{E(z)}{2\,\rho(z)[1+\sigma(z)]}\times$$

$$\times\left[\frac{\partial^2}{\partial x^2}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{\partial^2}{\partial x\,\partial y}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta\right]-K(z)\frac{\beta(z)}{\rho(z)}\int_0^\infty\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta-\frac{K(z)}{\rho(z)}\times$$

$$\times\frac{\partial^2}{\partial x\,\partial y}\int_0^\infty\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta-\frac{1}{\rho(z)}\frac{\partial^2}{\partial y^2}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta\left\{K(z)+\frac{5E(z)}{12[1+\sigma(z)]}\right\}-\frac{1}{2\,\rho(z)}\frac{\partial}{\partial z}\left\{\frac{E(z)}{1+\sigma(z)}\times\right.$$

$$\left.\times\left[\frac{\partial}{\partial z}\int_0^\infty\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{\partial}{\partial y}\int_0^\infty\int_0^\vartheta u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta\right]\right\}+u_{0y}-\frac{1}{\rho(z)}\frac{\partial^2}{\partial y\,\partial z}\int_0^\infty\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta\,\times$$

$$\times\left\{K(z)-\frac{E(z)}{6\,[1+\sigma(z)]}\right\}$$

$$u_z(x,y,z,t)=\frac{E(z)}{2\,[1+\sigma(z)]}\left[\frac{\partial^2}{\partial x^2}\int_0^\infty\int_0^\vartheta u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{\partial^2}{\partial y^2}\int_0^\infty\int_0^\vartheta u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{\partial^2}{\partial x\,\partial z}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta+\right.$$

$$\left.+\frac{\partial^2}{\partial y\,\partial z}\int_0^\infty\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta\right]\frac{1}{\rho(z)}+\frac{1}{\rho(z)}\frac{\partial}{\partial z}\left\{K(z)\left[\frac{\partial}{\partial x}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{\partial}{\partial y}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta+\right.\right.$$

$$\left.\left.+\frac{\partial}{\partial z}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta\right]\right\}+\frac{1}{6\rho(z)}\frac{\partial}{\partial z}\left\{\frac{E(z)}{1+\sigma(z)}\left[6\frac{\partial}{\partial z}\int_0^\infty\int_0^\vartheta u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta-\frac{\partial}{\partial x}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta-\right.\right.$$

$$\left.\left.-\frac{\partial}{\partial y}\int_0^\infty\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta-\frac{\partial}{\partial z}\int_0^\infty\int_0^\vartheta u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta\right]\right\}-K(z)\,\frac{\beta(z)}{\rho(z)}\frac{\partial}{\partial z}\int_0^\infty\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta+u_{0z}\,.$$

Spatio-temporal distributions of concentrations of charge carriers have been calculated by using of method of averaging of functional corrections [12-14]. To use the approach we replace required functions $n\,(x,y,z,t)$ and $p\,(x,y,z,t)$ in right sides of Eqs. (1) on their not yet known average values α_{1n} and α_{1p}. After the replacement we obtain equations for calculation the first-order approximations of required concentrations of charge carriers in the following form

$$\frac{\partial\,n_1(x,y,z,t)}{\partial\,t}=G-\alpha_{1n}\frac{\partial}{\partial\,x}\left\{\mu_n\frac{\partial[\varphi(x,y,z,t)+\varphi_h(x,y,z,t)]}{\partial\,x}\right\}-\alpha_{1n}\frac{\partial}{\partial\,y}\left\{\mu_n\frac{\partial[\varphi(x,y,z,t)+\varphi_h(x,y,z,t)]}{\partial\,y}\right\}-$$

$$-\alpha_{1n}\frac{\partial}{\partial\,z}\left\{\mu_n\frac{\partial[\varphi(x,y,z,t)+\varphi_h(x,y,z,t)]}{\partial\,z}\right\}+\alpha_{1n}\Omega\,L_z\left\{\frac{\partial}{\partial\,x}\left[\frac{D_{Sn}}{k\,T}\nabla_S\mu_h(x,y,z,t)\right]+\frac{\partial}{\partial\,y}\left[\frac{D_{Sn}}{k\,T}\nabla_S\mu_h(x,y,z,t)\right]\right\}-$$

$$-k_{np}\left(\alpha_{1n}\alpha_{1p}-n_0 p_0\right) \tag{9}$$

$$\frac{\partial p_1(x,y,z,t)}{\partial t}=G-\alpha_{1p}\frac{\partial}{\partial x}\left\{\mu_p\frac{\partial[\varphi(x,y,z,t)+\varphi_h(x,y,z,t)]}{\partial x}\right\}-\alpha_{1p}\frac{\partial}{\partial y}\left\{\mu_p\frac{\partial[\varphi(x,y,z,t)+\varphi_h(x,y,z,t)]}{\partial y}\right\}-$$

$$-\alpha_{1p}\frac{\partial}{\partial z}\left\{\mu_p\frac{\partial[\varphi(x,y,z,t)+\varphi_h(x,y,z,t)]}{\partial z}\right\}+\alpha_{1p}\Omega L_z\left\{\frac{\partial}{\partial x}\left[\frac{D_{Sp}}{kT}\nabla_S\mu_h(x,y,z,t)\right]+\frac{\partial}{\partial y}\left[\frac{D_{Sp}}{kT}\nabla_S\mu_h(x,y,z,t)\right]\right\}-$$

$$-k_{np}\left(\alpha_{1n}\alpha_{1p}-n_0 p_0\right).$$

Integration of both sides of Eqs. (9) on time t gives a possibility to obtain the first-order approximations of required concentrations in the final form

$$n_1(x,y,z,t)=\int_0^t G\,d\tau-\alpha_{1n}\frac{\partial}{\partial x}\int_0^t\mu_n\frac{\partial[\varphi(x,y,z,\tau)+\varphi_h(x,y,z,\tau)]}{\partial x}d\tau-\alpha_{1n}\frac{\partial}{\partial y}\int_0^t\mu_n\frac{\partial[\varphi(x,y,z,\tau)+\varphi_h(x,y,z,\tau)]}{\partial y}d\tau-$$

$$-\alpha_{1n}\frac{\partial}{\partial z}\int_0^t\mu_n\frac{\partial[\varphi(x,y,z,\tau)+\varphi_h(x,y,z,\tau)]}{\partial z}d\tau+\alpha_{1n}\Omega L_z\left[\frac{\partial}{\partial x}\int_0^t\frac{D_{Sn}}{kT}\nabla_S\mu_h(x,y,z,\tau)d\tau+\frac{\partial}{\partial y}\int_0^t\frac{D_{Sn}}{kT}\nabla_S\mu_h(x,y,z,\tau)d\tau\right]-$$

$$-k_{np}\int_0^t\left(\alpha_{1n}\alpha_{1p}-n_0 p_0\right)d\tau \tag{10}$$

$$p_1(x,y,z,t)=\int_0^t G\,d\tau-\alpha_{1p}\frac{\partial}{\partial x}\int_0^t\mu_p\frac{\partial[\varphi(x,y,z,\tau)+\varphi_h(x,y,z,\tau)]}{\partial x}d\tau-\alpha_{1p}\frac{\partial}{\partial y}\int_0^t\mu_p\frac{\partial[\varphi(x,y,z,\tau)+\varphi_h(x,y,z,\tau)]}{\partial y}d\tau-$$

$$-\alpha_{1p}\frac{\partial}{\partial z}\int_0^t\mu_p\frac{\partial[\varphi(x,y,z,\tau)+\varphi_h(x,y,z,\tau)]}{\partial z}d\tau+\alpha_{1p}\Omega L_z\left[\frac{\partial}{\partial x}\int_0^t\frac{D_{Sp}}{kT}\nabla_S\mu_h(x,y,z,\tau)d\tau+\frac{\partial}{\partial y}\int_0^t\frac{D_{Sp}}{kT}\nabla_S\mu_h(x,y,z,\tau)d\tau\right]-$$

$$-k_{np}\int_0^t\left(\alpha_{1n}\alpha_{1p}-n_0 p_0\right)d\tau\,.$$

Not yet known average values α_{1n} and α_{1p} could be determined by standard relations [12-14]

$$\alpha_{1n}=\int_0^{t_n}\int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{-L_z}^{L_z}n_1(x,y,z,t)\,dz\,dy\,dx\,dt\,,\;\alpha_{1p}=\int_0^{t_n}\int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{-L_z}^{L_z}p_1(x,y,z,t)\,dz\,dy\,dx\,dt\,, \tag{11}$$

where t_n is the observation time on charge carriers.

The second-order approximations of the required concentrations will be calculated framework standard replacement of functions $n\,(x,y,z,t)$ and $p\,(x,y,z,t)$ in right sides of Eqs. (1) on the following sums [12-14]: $n\,(x,y,z,t)\to\alpha_{1n}+n_1(x,y,z,t)$ и $p\,(x,y,z,t)\to\alpha_{1p}+p_1(x,y,z,t)$. Analogous procedure could be used for calculation of approximations of approximations with higher orders. After the above replacement we obtain equations for calculation of the considered the second-order approximations

$$\frac{\partial n_2(x,y,z,t)}{\partial t}=G+\frac{\partial}{\partial x}\left[D_n\frac{\partial n_1(x,y,z,t)}{\partial x}\right]+\frac{\partial}{\partial y}\left[D_n\frac{\partial n_1(x,y,z,t)}{\partial y}\right]+\frac{\partial}{\partial z}\left[D_n\frac{\partial n_1(x,y,z,t)}{\partial z}\right]-$$

$$-\frac{\partial}{\partial x}\left\{\mu_n[\alpha_{2n}+n_1(x,y,z,t)]\frac{\partial[\varphi(x,y,z,t)+\varphi_h(x,y,z,t)]}{\partial x}\right\}-\frac{\partial}{\partial y}\left\{\mu_n[\alpha_{2n}+n_1(x,y,z,t)]\frac{\partial[\varphi(x,y,z,t)+\varphi_h(x,y,z,t)]}{\partial y}\right\}-$$

$$-\frac{\partial}{\partial z}\left\{\mu_n[\alpha_{2n}+n_1(x,y,z,t)]\frac{\partial[\varphi(x,y,z,t)+\varphi_h(x,y,z,t)]}{\partial z}\right\}-k_{np}\left\{[\alpha_{2n}+n_1(x,y,z,t)][\alpha_{2p}+p_1(x,y,z,t)]-n_0p_0\right\}+$$

$$+\Omega\frac{\partial}{\partial x}\left\{\frac{D_{Sn}}{kT}\nabla_S\mu_h(x,y,z,t)\int_0^{L_z}[\alpha_{2n}+n_1(x,y,W,t)]\,dW\right\}+\Omega\frac{\partial}{\partial y}\left\{\frac{D_{Sn}}{kT}\nabla_S\mu_h(x,y,z,t)\int_0^{L_z}[\alpha_{2n}+n_1(x,y,W,t)]\,dW\right\}$$

(12)

$$\frac{\partial p_2(x,y,z,t)}{\partial t}=G+\frac{\partial}{\partial x}\left[D_p\frac{\partial p_1(x,y,z,t)}{\partial x}\right]+\frac{\partial}{\partial y}\left[D_p\frac{\partial p_1(x,y,z,t)}{\partial y}\right]+\frac{\partial}{\partial z}\left[D_p\frac{\partial p_1(x,y,z,t)}{\partial z}\right]-$$

$$-\frac{\partial}{\partial x}\left\{\mu_p\left[\alpha_{2p}+p_1(x,y,z,t)\right]\frac{\partial\left[\varphi(x,y,z,t)+\varphi_h(x,y,z,t)\right]}{\partial x}\right\}-\frac{\partial}{\partial y}\left\{\mu_p\left[\alpha_{2p}+p_1(x,y,z,t)\right]\frac{\partial\left[\varphi(x,y,z,t)+\varphi_h(x,y,z,t)\right]}{\partial y}\right\}-$$

$$-\frac{\partial}{\partial z}\left\{\mu_p\left[\alpha_{2p}+p_1(x,y,z,t)\right]\frac{\partial\left[\varphi(x,y,z,t)+\varphi_h(x,y,z,t)\right]}{\partial z}\right\}-k_{np}\left\{\left[\alpha_{2n}+n_1(x,y,z,t)\right]\left[\alpha_{2p}+p_1(x,y,z,t)\right]-n_0p_0\right\}+$$

$$+\Omega\frac{\partial}{\partial x}\left\{\frac{D_{Sp}}{kT}\nabla_S\mu_h(x,y,z,t)\int_0^{L_z}\left[\alpha_{2p}+p_1(x,y,W,t)\right]dW\right\}+\Omega\frac{\partial}{\partial y}\left\{\frac{D_{Sp}}{kT}\nabla_S\mu_h(x,y,z,t)\int_0^{L_z}\left[\alpha_{2p}+p_1(x,y,W,t)\right]dW\right\}.$$

Not yet known average values α_{2n} and α_{2p} could be calculated by using following standard relations [12-14]

$$\alpha_{2n}=\int_0^{t_n}\int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{-L_z}^{L_z}\left[n_2(x,y,z,t)-n_1(x,y,z,t)\right]dz\,dy\,dx\,dt,$$

$$\alpha_{2p}=\int_0^{t_n}\int_{-L_x}^{L_x}\int_{-L_y}^{L_y}\int_{-L_z}^{L_z}\left[p_2(x,y,z,t)-p_1(x,y,z,t)\right]dz\,dy\,dx\,dt, \quad (13)$$

where t_n is the observation time on charge carriers.

In this paper we calculate required concentrations of charge carriers and components of displacement vector by using the second-order approximations framework method of averaging of functional corrections. The approximation is usually enough good approximation to obtain qualitative conclusions and obtain some quantitative results. All analytical results were checked by comparison with results of numerical simulations.

3. Discussion

In this section we will analyze solution of system of Eqs. (1*a*) and compare it with experimental data. Most often in experimental works one can find voltage-current characteristics. Current density (let us consider current direction as parallel to axis *x*) in any point of the considered structure could be determined by the following relation [15]

$$J=e\left[D_n\frac{\partial n(x,y,z,t)}{\partial x}-D_p\frac{\partial p(x,y,z,t)}{\partial x}\right]-e\left[\mu_n n(x,y,z,t)+\mu_p p(x,y,z,t)\right]\frac{\partial\left[\varphi(x,y,z,t)+\varphi_h(x,y,z,t)\right]}{\partial x}.$$

$$J=e\left[D_n\frac{\partial n(x,y,z,t)}{\partial x}-D_p\frac{\partial p(x,y,z,t)}{\partial x}\right]-e\left[\mu_n n(x,y,z,t)+\mu_p p(x,y,z,t)\right]\frac{\partial\left[\varphi(x,y,z,t)+\varphi_h(x,y,z,t)\right]}{\partial x}.$$

(14)

Accounting of relation (5) in the relation (14) leads to the following result

$$J=e\left[D_n\frac{\partial n(x,y,z,t)}{\partial x}-D_p\frac{\partial p(x,y,z,t)}{\partial x}\right]-e\left[\mu_n n(x,y,z,t)+\mu_p p(x,y,z,t)\right]\frac{\partial\varphi_h(x,y,z,t)}{\partial x}-e\left(\varphi_k+U(t)+\frac{x-L_n}{L_p+L_n}\times\right.$$

$$\times\left[\mu_n n(x,y,z,t)+\mu_p p(x,y,z,t)\right]\left\{\varphi_k+U(t)-\frac{e}{\varepsilon\varepsilon_0}\int_{-L_p}^{L_n}(L_n-v)\left[p(v,y,z,t)-n(v,y,z,t)\right]dv\right\}-$$

$$\left.-\frac{e}{\varepsilon\varepsilon_0}\int_x^{L_n}(L_n-v)\left[p(v,y,z,t)-n(v,y,z,t)\right]dv\right). \quad (14a)$$

Figs. 4 show experimental voltage-current characteristics of *p*-*n*-junction in comparison with calculated in this paper one and with ideal one [15]. One can find from this figures, that voltage-current characteristics, calculated in this paper, has higher exactness in comparison with recently calculated one. It should be noted, that accounting of missmatch induced stress in heterostructure leads to forthcoming of voltage-current characteristics to the ordinate axis.

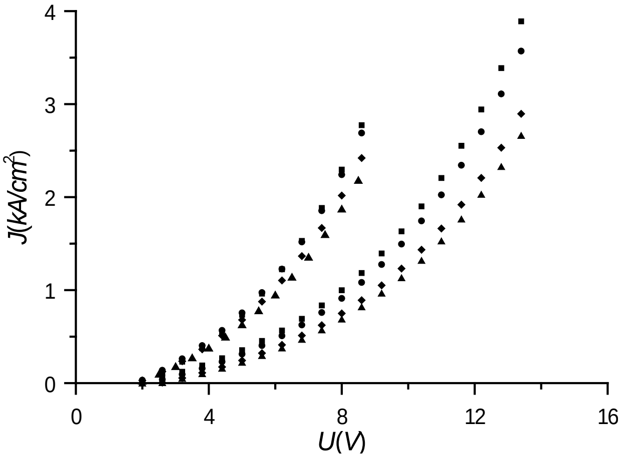

Fig. 4*a*. Direct branch of voltage-current characteristics of *p*-*n*-junction. Squares are the experimental data from [16]; circles are the calculated (in this paper) results with account missmatch induced stress; rhombus are the calculated (in this paper) results without accounting missmatch induced stress; triangles are the calculated in [15] results framework model of ideal voltage-current characteristic

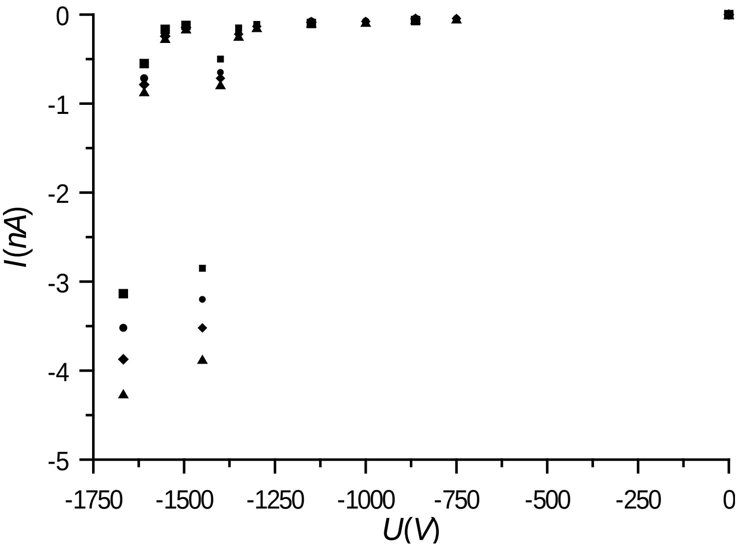

Fig. 4*b*. Inverse branch of voltage-current characteristics of *p*-*n*-junction. Squares are the experimental data from [16]; circles are the calculated (in this paper) results with account missmatch induced stress; rhombus are the calculated (in this paper) results without accounting missmatch induced stress; triangles are the calculated in [15] results framework model of ideal voltage-current characteristic

4. Conclusion

We consider a nonlinear model for analysis of current-voltage characteristic of a *p*-*n*-junction, which was manufactured in the framework of a heterostructure with specific configuration by diffusion or ion implantation. Based on result of analysis of the above model we compare voltage-current characteristics of *p*-*n*-junction, which were calculated by using the considered model, voltage-current characteristics of *p*-*n*-junction, which were calculated by using classical model of ideal *p*-*n*-junction and analogous experimental results.

5. References

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