

## RESEARCH ARTICLE

## On Optimization of Manufacturing of a Sense-amplifier Based Flip-flop

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### ABSTRACT

The paper describes an approach for increasing of density of field-effect heterotransistors in a sense-amplifier based flip-flop. To illustrate the approach, we consider manufacturing of an amplifier of power in a heterostructure with specific configuration. One shall dope some specific areas of the heterostructure by diffusion or ion implantation. After that, it should be done optimized annealing of radiation defects and/or dopant. We introduce an approach for decreasing of stress between layers of heterostructure. Furthermore, it has been considered an analytical approach for prognosis of heat and mass transport in heterostructures, which can be take into account mismatch-induced stress.

**Key words:** Broadband power amplifier, increasing of element integration rate, optimization of manufacturing

### INTRODUCTION

Now some electrical problems (to increase performance of solid-state electronic devices, to increase their reliability, and to increase density of integrated circuits elements: Transistors and diodes) are solving.<sup>[1-6]</sup> Increasing of performance could be obtained using materials, which have mobility of charge carriers with higher values.<sup>[7-10]</sup> Increasing of density of elements of integrated circuits could be obtained by optimized manufacturing of their elements in heterostructures with thin epitaxial layers.<sup>[3-5,11-15]</sup> In this situation, dimensions of elements of integrated circuits will be decreased. Another approach to decrease these dimensions is using microwave annealing and laser annealing of radiation defects and/or dopants.<sup>[16-18]</sup> In this paper, our aim is to formulate an approach to decrease dimensions of field-effect heterotransistors framework a broadband amplifier of power [Figure 1] framework a heterostructure with specific configuration (epitaxial layer/porous buffer layer/substrate and sections in the epitaxial layer, and manufactured using another materials).

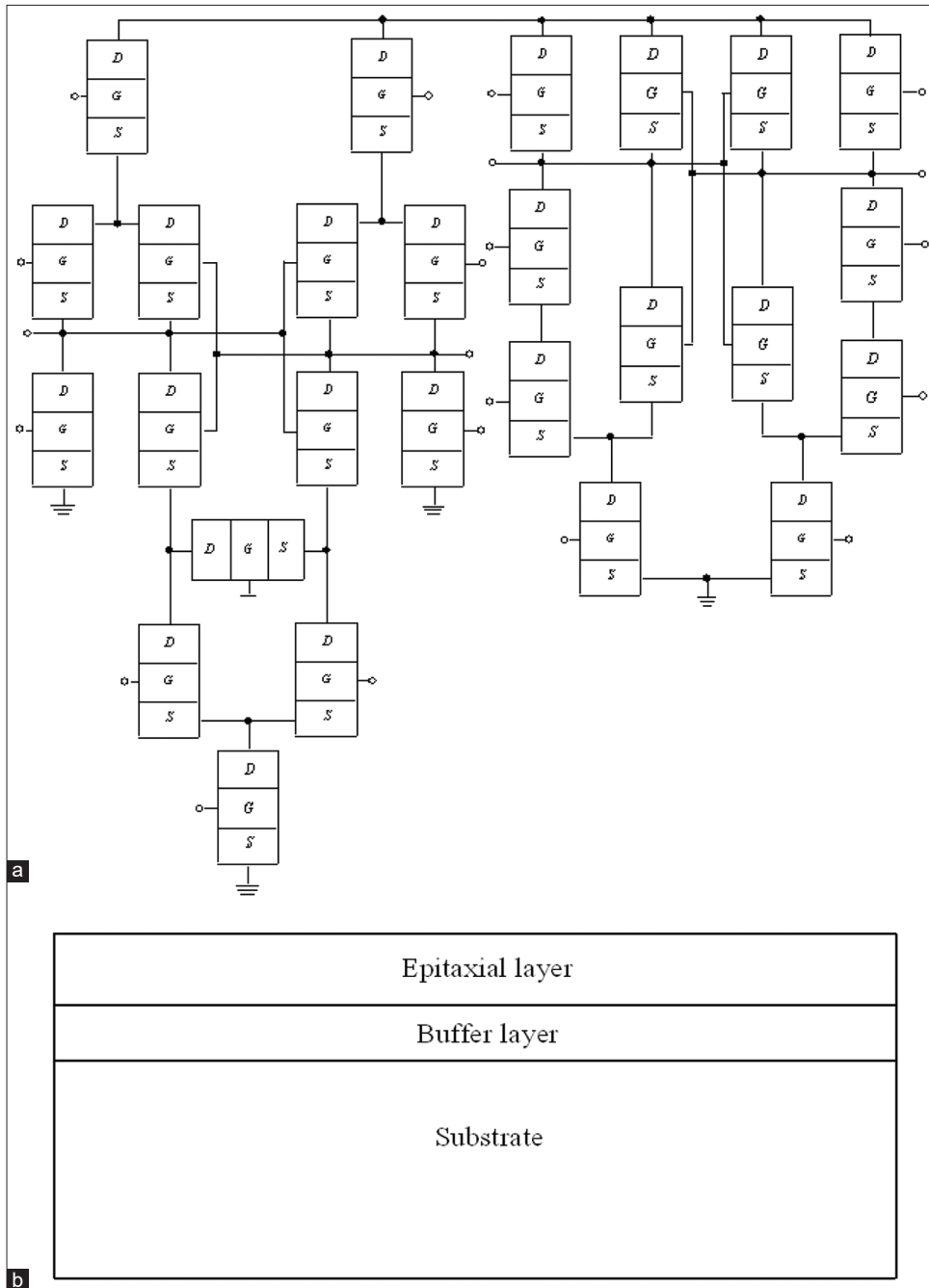
### Method of solution

Now let us analyze distribution of concentration of dopant in space and time in heterostructure from Figure 1. To determine the concentration, we solve the following second Fick's law.<sup>[1,20-23]</sup>

$$\frac{\partial C(x, y, z, t)}{\partial t} = \frac{\partial}{\partial x} \left[ D \frac{\partial C(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ D \frac{\partial C(x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[ D \frac{\partial C(x, y, z, t)}{\partial z} \right] +$$

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**Figure 1:** (a) Scheme of the amplifier, which considered in this paper.<sup>[19]</sup> (b) Considered heterostructure, which includes into itself epitaxial layers, buffer layer, and substrate

$$\Omega \frac{\partial}{\partial x} \left[ \frac{D_s}{kT} \nabla_s \mu_1(x, y, z, t) \int_0^{L_z} C(x, y, W, t) dW \right] +$$

$$\Omega \frac{\partial}{\partial y} \left[ \frac{D_s}{kT} \nabla_s \mu_1(x, y, z, t) \int_0^{L_z} C(x, y, W, t) dW \right] + \tag{1}$$

$$\frac{\partial}{\partial x} \left[ \frac{D_{Cs}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ \frac{D_{Cs}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[ \frac{D_{Cs}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial z} \right]$$

Conditions (initial and boundary) for this equation are following (these boundary conditions correspond to absents of dopant flow through external boundary of heterostructure; and the initial condition corresponds to distribution of dopant before starting of annealing).

$$\begin{aligned} \left. \frac{\partial C(x, y, z, t)}{\partial x} \right|_{x=0} = 0, \quad \left. \frac{\partial C(x, y, z, t)}{\partial x} \right|_{x=L_x} = 0, \quad \left. \frac{\partial C(x, y, z, t)}{\partial y} \right|_{y=0} = 0, \quad C(x, y, z, 0) = f_c(x, y, z), \\ \left. \frac{\partial C(x, y, z, t)}{\partial y} \right|_{x=L_y} = 0, \quad \left. \frac{\partial C(x, y, z, t)}{\partial z} \right|_{z=0} = 0, \quad \left. \frac{\partial C(x, y, z, t)}{\partial z} \right|_{x=L_z} = 0 \end{aligned} \quad (1a)$$

Function  $C(x, y, z, t)$  describes distribution of concentration of dopant in space and time; parameter  $\Omega$  mean volume of atom of dopant; symbol  $\nabla_s$  mean surficial gradient operator; function  $\int_0^{L_z} C(x, y, z, t) dz$  describes dopant surficial concentration on interface between layers of heterostructure (we consider: Z-axis is perpendicular to interface between heterostructure's layers); functions  $\mu_1(x, y, z, t)$  and  $\mu_2(x, y, z, t)$  describe distributions of chemical potentials in space and their dependences on temperature:  $\mu_1(x, y, z, t)$  accounting mismatch-induced stress in layers of heterostructure,  $\mu_2(x, y, z, t)$  accounting porosity of material; functions  $D(x, y, z, T)$  and  $D_s(x, y, z, T)$  describe distributions of coefficients of volumetric and surficial diffusions in space and their dependences on temperature. We used recently described approximations of dopant diffusions coefficients.<sup>[24-26]</sup>

$$\begin{aligned} D_C = D_L(x, y, z, T) \left[ 1 + \xi \frac{C^\gamma(x, y, z, t)}{P^\gamma(x, y, z, T)} \right] \left[ 1 + \zeta_1 \frac{V(x, y, z, t)}{V^*} + \zeta_2 \frac{V^2(x, y, z, t)}{(V^*)^2} \right], \\ D_S = D_{SL}(x, y, z, T) \left[ 1 + \xi_S \frac{C^\gamma(x, y, z, t)}{P^\gamma(x, y, z, T)} \right] \left[ 1 + \zeta_1 \frac{V(x, y, z, t)}{V^*} + \zeta_2 \frac{V^2(x, y, z, t)}{(V^*)^2} \right] \end{aligned} \quad (2)$$

Functions  $D_L(x, y, z, T)$  and  $D_{LS}(x, y, z, T)$  describe dependences of dopant diffusion coefficients on coordinate and temperature; parameter  $T$  describes temperature of annealing; function  $P(x, y, z, T)$  describes dependence of solubility of dopant on coordinate and temperature; value of parameter  $\gamma$  will be changed with changing of properties of materials and will be integer usually in the following interval  $\gamma \in [1, 3, 24]$  function  $V(x, y, z, t)$  describes distribution of radiation vacancies concentration in space and time with equilibrium distribution  $V^*$ . Distributions of point radiation defects concentration in space and time have been determined solutions of the following system of equations.<sup>[20-23, 25, 26]</sup>

$$\begin{aligned} \frac{\partial I(x, y, z, t)}{\partial t} = \frac{\partial}{\partial x} \left[ D_l(x, y, z, T) \frac{\partial I(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ D_l(x, y, z, T) \frac{\partial I(x, y, z, t)}{\partial y} \right] + \\ \frac{\partial}{\partial z} \left[ D_l(x, y, z, T) \frac{\partial I(x, y, z, t)}{\partial z} \right] - k_{l,l}(x, y, z, T) I^2(x, y, z, t) - k_{l,v}(x, y, z, T) \times \\ I(x, y, z, t) V(x, y, z, t) + \Omega \frac{\partial}{\partial x} \left[ \frac{D_{IS}}{kT} \nabla_s \mu(x, y, z, t) \int_0^{L_z} I(x, y, W, t) dW \right] + \\ \Omega \frac{\partial}{\partial y} \left[ \frac{D_{IS}}{kT} \nabla_s \mu(x, y, z, t) \int_0^{L_z} I(x, y, W, t) dW \right] + \frac{\partial}{\partial x} \left[ \frac{D_{IS}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial x} \right] + \end{aligned}$$

$$\frac{\partial}{\partial y} \left[ \frac{D_{IS}}{\bar{V}kT} \frac{\partial \mu_2(x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[ \frac{D_{IS}}{\bar{V}kT} \frac{\partial \mu_2(x, y, z, t)}{\partial z} \right] \quad (3)$$

$$\frac{\partial V(x, y, z, t)}{\partial t} = \frac{\partial}{\partial x} \left[ D_V(x, y, z, T) \frac{\partial V(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ D_V(x, y, z, T) \frac{\partial V(x, y, z, t)}{\partial y} \right] +$$

$$\frac{\partial}{\partial z} \left[ D_V(x, y, z, T) \frac{\partial V(x, y, z, t)}{\partial z} \right] - k_{V,V}(x, y, z, T) V^2(x, y, z, t) - k_{I,V}(x, y, z, T) \times$$

$$I(x, y, z, t) V(x, y, z, t) + \Omega \frac{\partial}{\partial x} \left[ \frac{D_{VS}}{kT} \nabla_S \mu(x, y, z, t) \int_0^{L_z} V(x, y, W, t) dW \right] +$$

$$\Omega \frac{\partial}{\partial y} \left[ \frac{D_{VS}}{kT} \nabla_S \mu(x, y, z, t) \int_0^{L_z} V(x, y, W, t) dW \right] + \frac{\partial}{\partial x} \left[ \frac{D_{VS}}{\bar{V}kT} \frac{\partial \mu_2(x, y, z, t)}{\partial x} \right] +$$

$$\frac{\partial}{\partial y} \left[ \frac{D_{VS}}{\bar{V}kT} \frac{\partial \mu_2(x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[ \frac{D_{VS}}{\bar{V}kT} \frac{\partial \mu_2(x, y, z, t)}{\partial z} \right]$$

Initial and boundary conditions for Eq. (3) could be written as

$$\left. \frac{\partial I(x, y, z, t)}{\partial x} \right|_{x=0} = 0, \quad \left. \frac{\partial I(x, y, z, t)}{\partial x} \right|_{x=L_x} = 0, \quad \left. \frac{\partial I(x, y, z, t)}{\partial y} \right|_{y=0} = 0,$$

$$\left. \frac{\partial I(x, y, z, t)}{\partial y} \right|_{y=L_y} = 0, \quad \left. \frac{\partial I(x, y, z, t)}{\partial z} \right|_{z=0} = 0, \quad \left. \frac{\partial I(x, y, z, t)}{\partial z} \right|_{z=L_z} = 0,$$

$$\left. \frac{\partial V(x, y, z, t)}{\partial x} \right|_{x=0} = 0, \quad \left. \frac{\partial V(x, y, z, t)}{\partial x} \right|_{x=L_x} = 0, \quad \left. \frac{\partial V(x, y, z, t)}{\partial y} \right|_{y=0} = 0, \quad (4)$$

$$\left. \frac{\partial V(x, y, z, t)}{\partial y} \right|_{y=L_y} = 0, \quad \left. \frac{\partial V(x, y, z, t)}{\partial z} \right|_{z=0} = 0, \quad \left. \frac{\partial V(x, y, z, t)}{\partial z} \right|_{z=L_z} = 0, \quad I(x, y, z, 0) =$$

$$f_I(x, y, z), \quad V(x, y, z, 0) = f_V(x, y, z), \quad V(x_1 + V_n t, y_1 + V_n t, z_1 + V_n t) = V_\infty \left( 1 + \frac{2 \ell \omega}{kT \sqrt{x_1^2 + y_1^2 + z_1^2}} \right)$$

Function  $I(x, y, z, t)$  describes distribution of concentration of radiation interstitials (equilibrium distribution  $I^*$ ) in space and time; functions  $D_I(x, y, z, T)$ ,  $D_V(x, y, z, T)$ ,  $D_{IS}(x, y, z, T)$ , and  $D_{VS}(x, y, z, T)$  describe dependences of volumetric and surficial diffusions coefficients of vacancies and interstitials on coordinates and temperature; terms  $I^2(x, y, z, t)$  and  $V^2(x, y, z, t)$  describe generation di-interstitials and divacancies (e.g., Vinetskiy and Kholodar<sup>[26]</sup> and appropriate references in this book); functions  $k_{I,V}(x, y, z, T)$ ,  $k_{I,I}(x, y, z, T)$ , and  $k_{V,I}(x, y, z, T)$  describe analogous dependences of parameters of recombination of point radiation defects and generation of their simplest complexes; parameter  $k$  corresponds to Boltzmann constant; parameter  $\omega$  is equal to  $a^3$ , where  $a$  describes interatomic distance; parameter  $\ell$

describes specific surface energy. To take into account the porosity of buffer layers we assume, that porous are approximately cylindrical with average values  $r = \sqrt{x_1^2 + y_1^2}$  and  $z_1$  before annealing.<sup>[23]</sup> With time small pores will decompose on vacancies. These vacancies will be absorbed by larger pores.<sup>[27]</sup> With the time volume of large pores decreasing due to absorbing these vacancies and became more spherical.<sup>[27]</sup> Distribution of concentration of vacancies in heterostructure, existing due to porosity, could be determined by summing on all pores, i.e.,

$$V(x, y, z, t) = \sum_{i=0}^l \sum_{j=0}^m \sum_{k=0}^n V_p(x + i\alpha, y + j\beta, z + k\chi, t), \quad R = \sqrt{x^2 + y^2 + z^2}$$

Parameters  $\alpha$ ,  $\beta$ , and  $\chi$  describe average distances between centers of pores in directions  $x$ ,  $y$ , and  $z$ , respectively, parameters  $l$ ,  $m$ , and  $n$  are the quantities of pores in appropriate directions.

Distributions of di-interstitials  $\Phi_I(x, y, z, t)$  and divacancies  $\Phi_V(x, y, z, t)$  in space and time have been calculated as solutions of the system of equations, which were presented below.<sup>[25,26]</sup>

$$\begin{aligned} \frac{\partial \Phi_I(x, y, z, t)}{\partial t} = & \frac{\partial}{\partial x} \left[ D_{\Phi_I}(x, y, z, T) \frac{\partial \Phi_I(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ D_{\Phi_I}(x, y, z, T) \frac{\partial \Phi_I(x, y, z, t)}{\partial y} \right] + \\ & \frac{\partial}{\partial z} \left[ D_{\Phi_I}(x, y, z, T) \frac{\partial \Phi_I(x, y, z, t)}{\partial z} \right] + \Omega \frac{\partial}{\partial x} \left[ \frac{D_{\Phi_I, S}}{kT} \nabla_s \mu_1(x, y, z, t) \int_0^{L_z} \Phi_I(x, y, W, t) dW \right] + \\ & \Omega \frac{\partial}{\partial y} \left[ \frac{D_{\Phi_I, S}}{kT} \nabla_s \mu_1(x, y, z, t) \int_0^{L_z} \Phi_I(x, y, W, t) dW \right] + k_{I, I}(x, y, z, T) I^2(x, y, z, t) + \\ & \frac{\partial}{\partial x} \left[ \frac{D_{\Phi_I, S}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ \frac{D_{\Phi_I, S}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[ \frac{D_{\Phi_I, S}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial z} \right] + \\ & k_I(x, y, z, T) I(x, y, z, t) \end{aligned} \tag{5}$$

$$\begin{aligned} \frac{\partial \Phi_V(x, y, z, t)}{\partial t} = & \frac{\partial}{\partial x} \left[ D_{\Phi_V}(x, y, z, T) \frac{\partial \Phi_V(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ D_{\Phi_V}(x, y, z, T) \frac{\partial \Phi_V(x, y, z, t)}{\partial y} \right] + \\ & \frac{\partial}{\partial z} \left[ D_{\Phi_V}(x, y, z, T) \frac{\partial \Phi_V(x, y, z, t)}{\partial z} \right] + \Omega \frac{\partial}{\partial x} \left[ \frac{D_{\Phi_V, S}}{kT} \nabla_s \mu_1(x, y, z, t) \int_0^{L_z} \Phi_V(x, y, W, t) dW \right] + \\ & \Omega \frac{\partial}{\partial y} \left[ \frac{D_{\Phi_V, S}}{kT} \nabla_s \mu_1(x, y, z, t) \int_0^{L_z} \Phi_V(x, y, W, t) dW \right] + k_{V, V}(x, y, z, T) V^2(x, y, z, t) + \\ & \frac{\partial}{\partial x} \left[ \frac{D_{\Phi_V, S}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ \frac{D_{\Phi_V, S}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[ \frac{D_{\Phi_V, S}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial z} \right] + \\ & k_V(x, y, z, T) V(x, y, z, t). \end{aligned}$$

Initial and boundary conditions for above equations takes the form

$$\left. \frac{\partial \Phi_I(x, y, z, t)}{\partial x} \right|_{x=0} = 0, \quad \left. \frac{\partial I(x, y, z, t)}{\partial x} \right|_{x=L_x} = 0, \quad \left. \frac{\partial I(x, y, z, t)}{\partial y} \right|_{y=0} = 0,$$

$$\begin{aligned} \left. \frac{\partial \Phi_I(x, y, z, t)}{\partial y} \right|_{y=L_y} = 0, \quad \left. \frac{\partial \Phi_I(x, y, z, t)}{\partial z} \right|_{z=0} = 0, \quad \left. \frac{\partial \Phi_I(x, y, z, t)}{\partial z} \right|_{z=L_z} = 0, \\ \left. \frac{\partial \Phi_V(x, y, z, t)}{\partial x} \right|_{x=0} = 0, \quad \left. \frac{\partial \Phi_V(x, y, z, t)}{\partial x} \right|_{x=L_x} = 0, \quad \left. \frac{\partial \Phi_V(x, y, z, t)}{\partial y} \right|_{y=0} = 0, \\ \left. \frac{\partial \Phi_V(x, y, z, t)}{\partial y} \right|_{y=L_y} = 0, \quad \left. \frac{\partial \Phi_V(x, y, z, t)}{\partial z} \right|_{z=0} = 0, \quad \left. \frac{\partial \Phi_V(x, y, z, t)}{\partial z} \right|_{z=L_z} = 0, \end{aligned} \quad (6)$$

$$\Phi_I(x, y, z, 0) = \phi_{\Phi_I}(x, y, z), \quad \Phi_V(x, y, z, 0) = \phi_{\Phi_V}(x, y, z).$$

Functions  $D_{\Phi_{IS}}(x, y, z, T)$ ,  $D_{\Phi_{VS}}(x, y, z, T)$ ,  $D_{\Phi_I}(x, y, z, T)$ , and  $D_{\Phi_V}(x, y, z, T)$  describe dependences of surficial and volumetric diffusions of complexes of radiation defects on coordinate and temperature; functions  $k_f(x, y, z, T)$  and  $k_v(x, y, z, T)$  describe analogous dependences of parameters of decay of the above complexes. We determined chemical potential  $\mu_1$  by the following relation.<sup>[20]</sup>

$$\mu_1 = E(z) W s_{ij} [u_{ij}(x, y, z, t) + u_{ji}(x, y, z, t)] / 2. \quad (7)$$

Function  $E(z)$  describes spatial dependences of Young modulus; value  $s_{ij}$  describes tensor of stress; value

$u_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$  describes tensor of deformation; values  $u_i$ , and  $u_j$  describe the displacement vector

$\vec{u}(x, y, z, t)$  components  $u_x(x, y, z, t)$ ,  $u_y(x, y, z, t)$ , and  $u_z(x, y, z, t)$ ;  $x, y, z$  are the coordinate  $x, y, z$ . The Eq. (3) could be transform to the following form

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

Value  $\sigma$  describes value of coefficient of Poisson; value  $\varepsilon_0 = (a_s - a_{EL}) / a_{EL}$  describes value of mismatch parameter, where parameters  $a_s, a_{EL}$  describes value of lattice distances in the considered substrate and the epitaxial layer, respectively; parameter  $K$  describes value of the uniform compression modulus; parameter  $\beta$  describes value of thermal expansion coefficient; parameter  $T_r$  describes value of equilibrium temperature, which we consider as room temperature. We consider components of displacement vector as solutions of the following equations.<sup>[21]</sup>

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

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

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

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

$\frac{\partial u_k(x, y, z, t)}{\partial x_k} - \beta(z)K(z)[T(x, y, z, t) - T_r]$ , where function  $\rho(z)$  describes the density of materials of

heterostructure and parameter,  $\delta_{ij}$  describes symbol of Kronecker. Accounting of the relation for  $s_{ij}$  in the last system of the equation leads to the following relation

$$\begin{aligned} \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\} \times \\ &\frac{\partial^2 u_y(x, y, z, t)}{\partial x \partial y} + \frac{E(z)}{2[1+\sigma(z)]} \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] \times \\ &\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] - \frac{\partial T(x, y, z, t)}{\partial y} \times \\ &K(z)\beta(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\} + \frac{\partial^2 u_y(x, y, z, t)}{\partial y^2} \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} + K(z) \frac{\partial^2 u_y(x, y, z, t)}{\partial x \partial y} \\ \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} + \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\} + \\ &\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\} - \\ &K(z)\beta(z) \frac{\partial T(x, y, z, t)}{\partial z}. \end{aligned} \tag{8}$$

Conditions for the above equations take the form

$$\frac{\partial \bar{u}(0, y, z, t)}{\partial x} = 0; \quad \frac{\partial \bar{u}(L_x, y, z, t)}{\partial x} = 0; \quad \frac{\partial \bar{u}(x, 0, z, t)}{\partial y} = 0; \quad \frac{\partial \bar{u}(x, L_y, z, t)}{\partial y} = 0;$$

$$\frac{\partial \bar{u}(x, y, 0, t)}{\partial z} = 0; \quad \frac{\partial \bar{u}(x, y, L_z, t)}{\partial z} = 0; \quad \bar{u}(x, y, z, 0) = \bar{u}_0; \quad \bar{u}(x, y, z, \infty) = \bar{u}.$$

We calculate dopant and radiation defects concentration distribution in space and time by the solution of the Eqs. (1), (3), and (5) using the standard method of averaging of function corrections.<sup>[28]</sup> First of all, we transform the Eqs. (1), (3), and (5) to the following form with accounting initial conditions of the above concentrations

$$\frac{\partial C(x, y, z, t)}{\partial t} = \frac{\partial}{\partial x} \left[ D \frac{\partial C(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ D \frac{\partial C(x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[ D \frac{\partial C(x, y, z, t)}{\partial z} \right] + \quad (1a)$$

$$+ f_c(x, y, z) \delta(t) + \frac{\partial}{\partial y} \left[ \frac{D_{CS}}{\bar{V} k T} \frac{\partial \mu_2(x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[ \frac{D_{CS}}{\bar{V} k T} \frac{\partial \mu_2(x, y, z, t)}{\partial z} \right] +$$

$$\frac{\partial}{\partial z} \left[ \frac{D_{CS}}{\bar{V} k T} \frac{\partial \mu_2(x, y, z, t)}{\partial z} \right] + \Omega \frac{\partial}{\partial x} \left[ \frac{D_s}{k T} \nabla_s \mu(x, y, z, t) \int_0^{L_z} C(x, y, W, t) dW \right] +$$

$$\Omega \frac{\partial}{\partial y} \left[ \frac{D_s}{k T} \nabla_s \mu(x, y, z, t) \int_0^{L_z} C(x, y, z, t) dW \right]$$

$$\frac{\partial I(x, y, z, t)}{\partial t} = \frac{\partial}{\partial x} \left[ D_I(x, y, z, T) \frac{\partial I(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ D_I(x, y, z, T) \frac{\partial I(x, y, z, t)}{\partial y} \right] +$$

$$\frac{\partial}{\partial z} \left[ D_I(x, y, z, T) \frac{\partial I(x, y, z, t)}{\partial z} \right] + \Omega \frac{\partial}{\partial x} \left[ \frac{D_{IS}}{k T} \nabla_s \mu_1(x, y, z, t) \int_0^{L_z} I(x, y, W, t) dW \right] +$$

$$\Omega \frac{\partial}{\partial y} \left[ \frac{D_{IS}}{k T} \nabla_s \mu_1(x, y, z, t) \int_0^{L_z} I(x, y, W, t) dW \right] - k_{I,I}(x, y, z, T) I^2(x, y, z, t) -$$

$$k_{I,V}(x, y, z, T) I(x, y, z, t) V(x, y, z, t) + f_I(x, y, z) \delta(t) \quad (3a)$$

$$\frac{\partial V(x, y, z, t)}{\partial t} = \frac{\partial}{\partial x} \left[ D_V(x, y, z, T) \frac{\partial V(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ D_V(x, y, z, T) \frac{\partial V(x, y, z, t)}{\partial y} \right] +$$

$$\frac{\partial}{\partial z} \left[ D_V(x, y, z, T) \frac{\partial V(x, y, z, t)}{\partial z} \right] + \Omega \frac{\partial}{\partial x} \left[ \frac{D_{VS}}{k T} \nabla_s \mu_1(x, y, z, t) \int_0^{L_z} V(x, y, W, t) dW \right] +$$

$$\Omega \frac{\partial}{\partial y} \left[ \frac{D_{VS}}{k T} \nabla_s \mu_1(x, y, z, t) \int_0^{L_z} V(x, y, W, t) dW \right] - k_{V,V}(x, y, z, T) I^2(x, y, z, t) -$$

$$k_{I,V}(x, y, z, T) I(x, y, z, t) V(x, y, z, t) + f_V(x, y, z) \delta(t)$$

$$\frac{\partial \Phi_I(x, y, z, t)}{\partial t} = \frac{\partial}{\partial x} \left[ D_{\Phi_I}(x, y, z, T) \frac{\partial \Phi_I(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ D_{\Phi_I}(x, y, z, T) \frac{\partial \Phi_I(x, y, z, t)}{\partial y} \right] +$$



$$\begin{aligned} & \frac{\partial}{\partial z} \left[ D_{\Phi_I} (x, y, z, T) \frac{\partial \Phi_I (x, y, z, t)}{\partial z} \right] + \Omega \frac{\partial}{\partial x} \left[ \frac{D_{\Phi_I, S}}{kT} \nabla_S \mu_1 (x, y, z, t) \int_0^{L_z} \Phi_I (x, y, W, t) dW \right] + \\ & \Omega \frac{\partial}{\partial y} \left[ \frac{D_{\Phi_I, S}}{kT} \nabla_S \mu_1 (x, y, z, t) \int_0^{L_z} \Phi_I (x, y, W, t) dW \right] + k_I (x, y, z, T) I (x, y, z, t) + \\ & \frac{\partial}{\partial x} \left[ \frac{D_{\Phi_I, S}}{\bar{V} kT} \frac{\partial \mu_2 (x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ \frac{D_{\Phi_I, S}}{\bar{V} kT} \frac{\partial \mu_2 (x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[ \frac{D_{\Phi_I, S}}{\bar{V} kT} \frac{\partial \mu_2 (x, y, z, t)}{\partial z} \right] + \\ & k_{I, I} (x, y, z, T) I^2 (x, y, z, t) + f_{\Phi_I} (x, y, z) \delta (t) \end{aligned} \tag{5a}$$

$$\begin{aligned} \frac{\partial \Phi_V (x, y, z, t)}{\partial t} &= \frac{\partial}{\partial x} \left[ D_{\Phi_V} (x, y, z, T) \frac{\partial \Phi_V (x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ D_{\Phi_V} (x, y, z, T) \frac{\partial \Phi_V (x, y, z, t)}{\partial y} \right] + \\ & \frac{\partial}{\partial z} \left[ D_{\Phi_V} (x, y, z, T) \frac{\partial \Phi_V (x, y, z, t)}{\partial z} \right] + \Omega \frac{\partial}{\partial x} \left[ \frac{D_{\Phi_V, S}}{kT} \nabla_S \mu_1 (x, y, z, t) \int_0^{L_z} \Phi_V (x, y, W, t) dW \right] + \\ & \Omega \frac{\partial}{\partial y} \left[ \frac{D_{\Phi_V, S}}{kT} \nabla_S \mu_1 (x, y, z, t) \int_0^{L_z} \Phi_V (x, y, W, t) dW \right] + k_V (x, y, z, T) V (x, y, z, t) + \\ & \frac{\partial}{\partial x} \left[ \frac{D_{\Phi_V, S}}{\bar{V} kT} \frac{\partial \mu_2 (x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ \frac{D_{\Phi_V, S}}{\bar{V} kT} \frac{\partial \mu_2 (x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[ \frac{D_{\Phi_V, S}}{\bar{V} kT} \frac{\partial \mu_2 (x, y, z, t)}{\partial z} \right] + \\ & k_{V, V} (x, y, z, T) V^2 (x, y, z, t) + f_{\Phi_V} (x, y, z) \delta (t) \end{aligned}$$

Now we consider not yet known average values  $a_{1r}$ , instead of radiation defects and dopant concentrations in right sides of Eqs. (1a), (3a), and (5a). The replacement gives a possibility to obtain equations for the first-order approximations of the required concentrations in the following form

$$\begin{aligned} \frac{\partial C_I (x, y, z, t)}{\partial t} &= \alpha_{1C} \Omega \frac{\partial}{\partial x} \left[ z \frac{D_S}{kT} \nabla_S \mu_1 (x, y, z, t) \right] + \alpha_{1C} \Omega \frac{\partial}{\partial y} \left[ z \frac{D_S}{kT} \nabla_S \mu_1 (x, y, z, t) \right] + \\ & f_C (x, y, z) \delta (t) + \frac{\partial}{\partial x} \left[ \frac{D_{CS}}{\bar{V} kT} \frac{\partial \mu_2 (x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ \frac{D_{CS}}{\bar{V} kT} \frac{\partial \mu_2 (x, y, z, t)}{\partial y} \right] + \\ & \frac{\partial}{\partial z} \left[ \frac{D_{CS}}{\bar{V} kT} \frac{\partial \mu_2 (x, y, z, t)}{\partial z} \right] \end{aligned} \tag{1b}$$

$$\begin{aligned} \frac{\partial I_1 (x, y, z, t)}{\partial t} &= \alpha_{1I} z \Omega \frac{\partial}{\partial x} \left[ \frac{D_{IS}}{kT} \nabla_S \mu (x, y, z, t) \right] + \alpha_{1I} \Omega \frac{\partial}{\partial y} \left[ z \frac{D_{IS}}{kT} \nabla_S \mu (x, y, z, t) \right] + \\ & \frac{\partial}{\partial x} \left[ \frac{D_{IS}}{\bar{V} kT} \frac{\partial \mu_2 (x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ \frac{D_{IS}}{\bar{V} kT} \frac{\partial \mu_2 (x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[ \frac{D_{IS}}{\bar{V} kT} \frac{\partial \mu_2 (x, y, z, t)}{\partial z} \right] + \end{aligned}$$

$$f_I(x, y, z)\delta(t) - \alpha_{1I}^2 k_{I,I}(x, y, z, T) - \alpha_{1I}\alpha_{1V} k_{I,V}(x, y, z, T) \tag{3b}$$

$$\frac{\partial V_1(x, y, z, t)}{\partial t} = \alpha_{1V} z \Omega \frac{\partial}{\partial x} \left[ \frac{D_{VS}}{kT} \nabla_S \mu_1(x, y, z, t) \right] + \alpha_{1V} \Omega \frac{\partial}{\partial y} \left[ z \frac{D_{VS}}{kT} \nabla_S \mu_1(x, y, z, t) \right] +$$

$$\frac{\partial}{\partial x} \left[ \frac{D_{VS}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ \frac{D_{VS}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[ \frac{D_{VS}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial z} \right] +$$

$$f_V(x, y, z)\delta(t) - \alpha_{1V}^2 k_{V,V}(x, y, z, T) - \alpha_{1I}\alpha_{1V} k_{I,V}(x, y, z, T)$$

$$\frac{\partial \Phi_{1I}(x, y, z, t)}{\partial t} = \alpha_{1\Phi_I} z \Omega \frac{\partial}{\partial x} \left[ \frac{D_{\Phi_I S}}{kT} \nabla_S \mu_1(x, y, z, t) \right] + \alpha_{1\Phi_I} z \Omega \frac{\partial}{\partial y} \left[ \frac{D_{\Phi_I S}}{kT} \nabla_S \mu_1(x, y, z, t) \right] +$$

$$\frac{\partial}{\partial x} \left[ \frac{D_{\Phi_I S}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ \frac{D_{\Phi_I S}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[ \frac{D_{\Phi_I S}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial z} \right] +$$

$$f_{\Phi_I}(x, y, z)\delta(t) + k_I(x, y, z, T)I(x, y, z, t) + k_{I,I}(x, y, z, T)I^2(x, y, z, t) \tag{5b}$$

$$\frac{\partial \Phi_{1V}(x, y, z, t)}{\partial t} = \alpha_{1\Phi_V} \bar{z} \Omega \frac{\partial}{\partial x} \left[ \frac{D_{\Phi_V S}}{kT} \nabla_S \mu_1(x, y, z, t) \right] + \alpha_{1\Phi_V} \bar{z} \Omega \frac{\partial}{\partial y} \left[ \frac{D_{\Phi_V S}}{kT} \nabla_S \mu_1(x, y, z, t) \right] +$$

$$\frac{\partial}{\partial x} \left[ \frac{D_{\Phi_V S}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ \frac{D_{\Phi_V S}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[ \frac{D_{\Phi_V S}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial z} \right] +$$

$$f_{\Phi_V}(x, y, z)\delta(t) + k_V(x, y, z, T)V(x, y, z, t) + k_{V,V}(x, y, z, T)V^2(x, y, z, t)$$

Integration of the left and right sides of the Eqs. (1b), (3b), and (5b) on time gives us the possibility to obtain relations for above approximation in this form

$$C_1(x, y, z, t) = \alpha_{1C} \Omega \frac{\partial}{\partial x} \int_0^t D_{SL}(x, y, z, T) \frac{z}{kT} \left[ 1 + \zeta_1 \frac{V(x, y, z, \tau)}{V^*} + \zeta_2 \frac{V^2(x, y, z, \tau)}{(V^*)^2} \right] \times$$

$$\nabla_S \mu_1(x, y, z, \tau) \left[ 1 + \frac{\xi_S \alpha_{1C}^r}{P^r(x, y, z, T)} \right] d\tau \left\} + \alpha_{1C} \frac{\partial}{\partial y} \int_0^t D_{SL}(x, y, z, T) \left[ 1 + \frac{\xi_S \alpha_{1C}^r}{P^r(x, y, z, T)} \right] +$$

$$\Omega \nabla_S \mu_1(x, y, z, \tau) \frac{z}{kT} \left[ 1 + \zeta_1 \frac{V(x, y, z, \tau)}{V^*} + \zeta_2 \frac{V^2(x, y, z, \tau)}{(V^*)^2} \right] d\tau + \frac{\partial}{\partial x} \int_0^t \frac{D_{CS}}{\bar{V} kT} \times$$

$$\frac{\partial \mu_2(x, y, z, \tau)}{\partial x} d\tau + \frac{\partial}{\partial y} \int_0^t \frac{D_{CS}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, \tau)}{\partial y} d\tau + \frac{\partial}{\partial z} \int_0^t \frac{D_{CS}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, \tau)}{\partial z} d\tau +$$

$$f_C(x, y, z) \tag{1c}$$

$$I_1(x, y, z, t) = \alpha_{I1} z \Omega \frac{\partial}{\partial x} \int_0^t \frac{D_{IS}}{kT} \nabla_S \mu_1(x, y, z, \tau) d\tau + \alpha_{I1} z \Omega \frac{\partial}{\partial y} \int_0^t \frac{D_{IS}}{kT} \nabla_S \mu_1(x, y, z, \tau) d\tau +$$

$$\frac{\partial}{\partial x} \int_0^t \frac{D_{IS}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial x} d\tau + \frac{\partial}{\partial y} \int_0^t \frac{D_{IS}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial y} d\tau + \frac{\partial}{\partial z} \int_0^t \frac{D_{IS}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial z} d\tau +$$

$$f_I(x, y, z) - \alpha_{I1}^2 \int_0^t k_{I,I}(x, y, z, T) d\tau - \alpha_{I1} \alpha_{IV} \int_0^t k_{I,V}(x, y, z, T) d\tau \tag{3c}$$

$$V_1(x, y, z, t) = \alpha_{IV} z \Omega \frac{\partial}{\partial x} \int_0^t \frac{D_{IS}}{kT} \nabla_S \mu_1(x, y, z, \tau) d\tau + \alpha_{IV} z \Omega \frac{\partial}{\partial y} \int_0^t \frac{D_{IS}}{kT} \nabla_S \mu_1(x, y, z, \tau) d\tau +$$

$$\frac{\partial}{\partial x} \int_0^t \frac{D_{VS}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial x} d\tau + \frac{\partial}{\partial y} \int_0^t \frac{D_{VS}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial y} d\tau + \frac{\partial}{\partial z} \int_0^t \frac{D_{VS}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, t)}{\partial z} d\tau +$$

$$f_V(x, y, z) - \alpha_{IV}^2 \int_0^t k_{V,V}(x, y, z, T) d\tau - \alpha_{IV} \alpha_{IV} \int_0^t k_{I,V}(x, y, z, T) d\tau$$

$$\Phi_{I1}(x, y, z, t) = \alpha_{1\Phi_I} z \Omega \frac{\partial}{\partial x} \int_0^t \frac{D_{\Phi_I S}}{kT} \nabla_S \mu_1(x, y, z, \tau) d\tau + \Omega \frac{\partial}{\partial x} \int_0^t \frac{D_{\Phi_I S}}{kT} \nabla_S \mu_1(x, y, z, \tau) d\tau \times$$

$$\alpha_{1\Phi_I} z + f_{\Phi_I}(x, y, z) + \frac{\partial}{\partial x} \int_0^t \frac{D_{\Phi_I S}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, \tau)}{\partial x} d\tau + \frac{\partial}{\partial y} \int_0^t \frac{D_{\Phi_I S}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, \tau)}{\partial y} d\tau +$$

$$\frac{\partial}{\partial z} \int_0^t \frac{D_{\Phi_I S}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, \tau)}{\partial z} d\tau + \int_0^t k_I(x, y, z, T) I(x, y, z, \tau) d\tau +$$

$$\int_0^t k_{I,I}(x, y, z, T) I^2(x, y, z, \tau) d\tau$$

$$\Phi_{IV}(x, y, z, t) = \alpha_{1\Phi_V} z \Omega \frac{\partial}{\partial x} \int_0^t \frac{D_{\Phi_V S}}{kT} \nabla_S \mu_1(x, y, z, \tau) d\tau + \Omega \frac{\partial}{\partial x} \int_0^t \frac{D_{\Phi_V S}}{kT} \nabla_S \mu_1(x, y, z, \tau) d\tau \times$$

$$\alpha_{1\Phi_V} z + f_{\Phi_V}(x, y, z) + \frac{\partial}{\partial x} \int_0^t \frac{D_{\Phi_V S}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, \tau)}{\partial x} d\tau + \frac{\partial}{\partial y} \int_0^t \frac{D_{\Phi_V S}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, \tau)}{\partial y} d\tau +$$

$$\frac{\partial}{\partial z} \int_0^t \frac{D_{\Phi_V S}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, \tau)}{\partial z} d\tau + \int_0^t k_V(x, y, z, T) V(x, y, z, \tau) d\tau +$$

$$\int_0^t k_{V,V}(x, y, z, T) V^2(x, y, z, \tau) d\tau.$$

Following standard relation gives a possibility to calculate average values of the first-order approximations of dopant and radiation defects concentrations.<sup>[28]</sup>

$$\alpha_{1\rho} = \frac{1}{\Theta L_x L_y L_z} \int_0^{\Theta} \int_0^{L_x} \int_0^{L_y} \int_0^{L_z} \rho_1(x, y, z, t) dz dy dx dt \tag{9}$$

Substitution of the above first-order approximations into relation Eqs. (9) leads to the following results

$$\alpha_{1C} = \frac{1}{L_x L_y L_z} \int_0^{L_x} \int_0^{L_y} \int_0^{L_z} f_C(x, y, z) dz dy dx, \quad \alpha_{1I} = \sqrt{\frac{(a_3 + A)^2}{4a_4^2} - 4 \left( B + \frac{\Theta a_3 B + \Theta^2 L_x L_y L_z a_1}{a_4} \right)} - \frac{a_3 + A}{4a_4},$$

$$\alpha_{1V} = \frac{1}{S_{IV00}} \left[ \frac{\Theta}{\alpha_{1I}} \int_0^{L_x} \int_0^{L_y} \int_0^{L_z} f_I(x, y, z) dz dy dx - \alpha_{1I} S_{II00} - \Theta L_x L_y L_z \right].$$

Here  $S_{\rho\rho ij} = \int_0^{\Theta} (\Theta - t) \int_0^{L_x} \int_0^{L_y} \int_0^{L_z} k_{\rho,\rho}(x, y, z, T) I_1^i(x, y, z, t) V_1^j(x, y, z, t) dz dy dx dt$ ,  $a_4 = S_{II00} \times$

$$\left( S_{IV00}^2 - S_{II00} S_{VV00} \right), \quad a_3 = S_{IV00} S_{II00} + S_{IV00}^2 - S_{II00} S_{VV00}, \quad a_2 = \int_0^{L_x} \int_0^{L_y} \int_0^{L_z} f_V(x, y, z) dz dy dx \times$$

$$S_{IV00} S_{IV00}^2 + S_{IV00} \Theta L_x^2 L_y^2 L_z^2 + 2 S_{VV00} S_{II00} \int_0^{L_x} \int_0^{L_y} \int_0^{L_z} f_I(x, y, z) dz dy dx - \Theta L_x^2 L_y^2 L_z^2 S_{VV00} -$$

$$S_{IV00}^2 \int_0^{L_x} \int_0^{L_y} \int_0^{L_z} f_I(x, y, z) dz dy dx, \quad a_1 = S_{IV00} \int_0^{L_x} \int_0^{L_y} \int_0^{L_z} f_I(x, y, z) dz dy dx, \quad a_0 = S_{VV00} \times$$

$$\left[ \int_0^{L_x} \int_0^{L_y} \int_0^{L_z} f_I(x, y, z) dz dy dx \right]^2, \quad A = \sqrt{8y + \Theta^2 \frac{a_3^2}{a_4^2} - 4\Theta \frac{a_2}{a_4}}, \quad B = \frac{\Theta a_2}{6a_4} + \sqrt[3]{\sqrt{q^2 + p^3} - q -}$$

$$\sqrt[3]{\sqrt{q^2 + p^3} + q}, \quad q = \frac{\Theta^3 a_2}{24 a_4^2} \left( 4a_0 - \Theta L_x L_y L_z \frac{a_1 a_3}{a_4} \right) - \Theta^2 \frac{a_0}{8 a_4^2} \left( 4\Theta a_2 - \Theta^2 \frac{a_3^2}{a_4} \right) - \frac{\Theta^3 a_2^3}{54 a_4^3} -$$

$$L_x^2 L_y^2 L_z^2 \frac{\Theta^4 a_1^2}{8 a_4^2}, \quad p = \Theta^2 \frac{4a_0 a_4 - \Theta L_x L_y L_z a_1 a_3}{12 a_4^2} - \frac{\Theta a_2}{18 a_4},$$

$$\alpha_{1\Phi_I} = \frac{R_{I1}}{\Theta L_x L_y L_z} + \frac{S_{II20}}{\Theta L_x L_y L_z} + \frac{1}{L_x L_y L_z} \int_0^{L_x} \int_0^{L_y} \int_0^{L_z} f_{\Phi_I}(x, y, z) dz dy dx$$

$$\alpha_{1\Phi_V} = \frac{R_{V1}}{\Theta L_x L_y L_z} + \frac{S_{VV20}}{\Theta L_x L_y L_z} + \frac{1}{L_x L_y L_z} \int_0^{L_x} \int_0^{L_y} \int_0^{L_z} f_{\Phi_V}(x, y, z) dz dy dx.$$

Here  $R_{\rho_i} = \int_0^{\Theta} (\Theta - t) \int_0^{L_x} \int_0^{L_y} \int_0^{L_z} k_I(x, y, z, T) I_1^i(x, y, z, t) dz dy dx dt$ .

Now, we calculate approximations with the second and higher ( $n$ -th) orders of considered concentrations using the method of averaging of function corrections in the classical form.<sup>[28]</sup> The considered procedure leads to the replacement of considered concentrations on the right sides of Eqs. (1c), (3c), and (5c) on the following sum  $\alpha_{nr} + \rho_{n-1}(x, y, z, t)$ . In this situation, one can obtain the following equations for the second-order approximations of the above concentrations

$$\begin{aligned} \frac{\partial C_2(x, y, z, t)}{\partial t} &= \frac{\partial}{\partial x} \left\{ \left[ 1 + \xi \frac{[\alpha_{2c} + C_1(x, y, z, t)]^{\gamma}}{P^{\gamma}(x, y, z, T)} \right] \left[ 1 + \varsigma_1 \frac{V(x, y, z, t)}{V^*} + \varsigma_2 \frac{V^2(x, y, z, t)}{(V^*)^2} \right] \right\} \times \\ &\times D_L(x, y, z, T) \frac{\partial C_1(x, y, z, t)}{\partial x} + \frac{\partial}{\partial y} \left\{ \left[ 1 + \varsigma_1 \frac{V(x, y, z, t)}{V^*} + \varsigma_2 \frac{V^2(x, y, z, t)}{(V^*)^2} \right] \frac{\partial C_1(x, y, z, t)}{\partial y} \right\} \times \\ &D_L(x, y, z, T) \left\{ 1 + \xi \frac{[\alpha_{2c} + C_1(x, y, z, t)]^{\gamma}}{P^{\gamma}(x, y, z, T)} \right\} + \frac{\partial}{\partial z} \left\{ \left[ 1 + \varsigma_1 \frac{V(x, y, z, t)}{V^*} + \varsigma_2 \frac{V^2(x, y, z, t)}{(V^*)^2} \right] \right\} \times \\ &D_L(x, y, z, T) \frac{\partial C_1(x, y, z, t)}{\partial z} \left\{ 1 + \xi \frac{[\alpha_{2c} + C_1(x, y, z, t)]^{\gamma}}{P^{\gamma}(x, y, z, T)} \right\} + f_c(x, y, z) \delta(t) + \\ &\frac{\partial}{\partial x} \left[ \frac{D_{CS}}{\bar{V} k T} \frac{\partial \mu_2(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ \frac{D_{CS}}{\bar{V} k T} \frac{\partial \mu_2(x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[ \frac{D_{CS}}{\bar{V} k T} \frac{\partial \mu_2(x, y, z, t)}{\partial z} \right] + \\ &\Omega \frac{\partial}{\partial x} \left\{ \frac{D_S}{k T} \nabla_S \mu_1(x, y, z, t) \int_0^{L_z} [\alpha_{2c} + C(x, y, W, t)] dW \right\} + \\ &\Omega \frac{\partial}{\partial y} \left\{ \frac{D_S}{k T} \nabla_S \mu_1(x, y, z, t) \int_0^{L_z} [\alpha_{2c} + C(x, y, W, t)] dW \right\} \tag{1d} \\ \frac{\partial I_2(x, y, z, t)}{\partial t} &= \frac{\partial}{\partial x} \left[ D_I(x, y, z, T) \frac{\partial I_1(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ D_I(x, y, z, T) \frac{\partial I_1(x, y, z, t)}{\partial y} \right] + \\ &\frac{\partial}{\partial z} \left[ D_I(x, y, z, T) \frac{\partial I_1(x, y, z, t)}{\partial z} \right] - k_{I,I}(x, y, z, T) [\alpha_{I,I} + I_1(x, y, z, t)]^2 - k_{I,V}(x, y, z, T) \times \\ &[\alpha_{I,I} + I_1(x, y, z, t)] [\alpha_{I,V} + V_1(x, y, z, t)] + \Omega \frac{\partial}{\partial x} \left\{ \nabla_S \mu(x, y, z, t) \int_0^{L_z} [\alpha_{2I} + I_1(x, y, W, t)] dW \right\} \times \\ &\frac{D_{IS}}{k T} \left\{ + \Omega \frac{\partial}{\partial y} \left\{ \frac{D_{IS}}{k T} \nabla_S \mu(x, y, z, t) \int_0^{L_z} [\alpha_{2I} + I_1(x, y, W, t)] dW \right\} + \frac{\partial}{\partial x} \int_0^{L_z} \frac{\partial \mu_2(x, y, z, t)}{\partial x} \right\} \times \end{aligned}$$

$$\frac{D_{IS}}{\bar{V}kT}d\tau + \frac{\partial}{\partial y} \int_0^t \frac{D_{IS}}{\bar{V}kT} \frac{\partial \mu_2(x,y,z,t)}{\partial y} d\tau + \frac{\partial}{\partial z} \int_0^t \frac{D_{IS}}{\bar{V}kT} \frac{\partial \mu_2(x,y,z,t)}{\partial z} d\tau \quad (3d)$$

$$\begin{aligned} \frac{\partial V_2(x,y,z,t)}{\partial t} &= \frac{\partial}{\partial x} \left[ D_V(x,y,z,T) \frac{\partial V_1(x,y,z,t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ D_V(x,y,z,T) \frac{\partial V_1(x,y,z,t)}{\partial y} \right] + \\ &\frac{\partial}{\partial z} \left[ D_V(x,y,z,T) \frac{\partial V_1(x,y,z,t)}{\partial z} \right] - k_{V,V}(x,y,z,T) [\alpha_{1V} + V_1(x,y,z,t)]^2 - k_{I,V}(x,y,z,T) \times \\ &[\alpha_{1I} + I_1(x,y,z,t)] [\alpha_{1V} + V_1(x,y,z,t)] + \Omega \frac{\partial}{\partial x} \left\{ \nabla_S \mu(x,y,z,t) \int_0^{L_z} [\alpha_{2V} + V_1(x,y,W,t)] dW \times \right. \\ &\left. \frac{D_{VS}}{kT} \right\} + \Omega \frac{\partial}{\partial y} \left\{ \frac{D_{VS}}{kT} \nabla_S \mu(x,y,z,t) \int_0^{L_z} [\alpha_{2V} + V_1(x,y,W,t)] dW \right\} + \frac{\partial}{\partial x} \int_0^t \frac{\partial \mu_2(x,y,z,t)}{\partial x} \times \\ &\frac{D_{VS}}{\bar{V}kT} d\tau + \frac{\partial}{\partial y} \int_0^t \frac{D_{VS}}{\bar{V}kT} \frac{\partial \mu_2(x,y,z,t)}{\partial y} d\tau + \frac{\partial}{\partial z} \int_0^t \frac{D_{VS}}{\bar{V}kT} \frac{\partial \mu_2(x,y,z,t)}{\partial z} d\tau \\ \frac{\partial \Phi_{2I}(x,y,z,t)}{\partial t} &= \frac{\partial}{\partial x} \left[ D_{\Phi_I}(x,y,z,T) \frac{\partial \Phi_{1I}(x,y,z,t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ D_{\Phi_I}(x,y,z,T) \frac{\partial \Phi_{1I}(x,y,z,t)}{\partial y} \right] + \\ &\Omega \frac{\partial}{\partial x} \left\{ \frac{D_{\Phi_I S}}{kT} \nabla_S \mu(x,y,z,t) \int_0^{L_z} [\alpha_{2\Phi_I} + \Phi_{1I}(x,y,W,t)] dW \right\} + k_{I,I}(x,y,z,T) I^2(x,y,z,t) + \\ &\Omega \frac{\partial}{\partial y} \left\{ \frac{D_{\Phi_I S}}{kT} \nabla_S \mu(x,y,z,t) \int_0^{L_z} [\alpha_{2\Phi_I} + \Phi_{1I}(x,y,W,t)] dW \right\} + k_I(x,y,z,T) I(x,y,z,t) + \\ &\frac{\partial}{\partial x} \left[ \frac{D_{\Phi_I S}}{\bar{V}kT} \frac{\partial \mu_2(x,y,z,t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ \frac{D_{\Phi_I S}}{\bar{V}kT} \frac{\partial \mu_2(x,y,z,t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[ \frac{D_{\Phi_I S}}{\bar{V}kT} \frac{\partial \mu_2(x,y,z,t)}{\partial z} \right] + \\ &\frac{\partial}{\partial z} \left[ D_{\Phi_I}(x,y,z,T) \frac{\partial \Phi_{1I}(x,y,z,t)}{\partial z} \right] + f_{\Phi_I}(x,y,z) \delta(t) \end{aligned} \quad (5d)$$

$$\begin{aligned} \frac{\partial \Phi_{2V}(x,y,z,t)}{\partial t} &= \frac{\partial}{\partial x} \left[ D_{\Phi_V}(x,y,z,T) \frac{\partial \Phi_{1V}(x,y,z,t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ D_{\Phi_V}(x,y,z,T) \frac{\partial \Phi_{1V}(x,y,z,t)}{\partial y} \right] + \\ &\Omega \frac{\partial}{\partial x} \left\{ \frac{D_{\Phi_V S}}{kT} \nabla_S \mu(x,y,z,t) \int_0^{L_z} [\alpha_{2\Phi_V} + \Phi_{1V}(x,y,W,t)] dW \right\} + k_{V,V}(x,y,z,T) V^2(x,y,z,t) + \\ &\Omega \frac{\partial}{\partial y} \left\{ \frac{D_{\Phi_V S}}{kT} \nabla_S \mu(x,y,z,t) \int_0^{L_z} [\alpha_{2\Phi_V} + \Phi_{1V}(x,y,W,t)] dW \right\} + k_V(x,y,z,T) V(x,y,z,t) + \end{aligned}$$

$$\frac{\partial}{\partial x} \left[ \frac{D_{\Phi_r S}}{\bar{V} k T} \frac{\partial \mu_2(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ \frac{D_{\Phi_r S}}{\bar{V} k T} \frac{\partial \mu_2(x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[ \frac{D_{\Phi_r S}}{\bar{V} k T} \frac{\partial \mu_2(x, y, z, t)}{\partial z} \right] +$$

$$\frac{\partial}{\partial z} \left[ D_{\Phi_r} (x, y, z, T) \frac{\partial \Phi_{IV}(x, y, z, t)}{\partial z} \right] + f_{\Phi_r} (x, y, z) \delta(t).$$

The above equations could be solved by the integration of both sides of the above equations on time. After this integration one can be obtained

$$C_2(x, y, z, t) = \frac{\partial}{\partial x} \int_0^t \left\{ 1 + \xi \frac{[\alpha_{2C} + C_1(x, y, z, \tau)]^\gamma}{P^\gamma(x, y, z, T)} \right\} \left[ 1 + \varsigma_1 \frac{V(x, y, z, \tau)}{V^*} + \varsigma_2 \frac{V^2(x, y, z, \tau)}{(V^*)^2} \right] \times$$

$$D_L(x, y, z, T) \frac{\partial C_1(x, y, z, \tau)}{\partial x} d\tau + \frac{\partial}{\partial y} \int_0^t D_L(x, y, z, T) \left[ 1 + \varsigma_1 \frac{V(x, y, z, \tau)}{V^*} + \varsigma_2 \frac{V^2(x, y, z, \tau)}{(V^*)^2} \right] \times$$

$$\frac{\partial C_1(x, y, z, \tau)}{\partial y} \left\{ 1 + \xi \frac{[\alpha_{2C} + C_1(x, y, z, \tau)]^\gamma}{P^\gamma(x, y, z, T)} \right\} + \frac{\partial}{\partial z} \int_0^t \left[ 1 + \varsigma_1 \frac{V(x, y, z, \tau)}{V^*} + \varsigma_2 \frac{V^2(x, y, z, \tau)}{(V^*)^2} \right] \times$$

$$D_L(x, y, z, T) \frac{\partial C_1(x, y, z, \tau)}{\partial z} \left\{ 1 + \xi \frac{[\alpha_{2C} + C_1(x, y, z, \tau)]^\gamma}{P^\gamma(x, y, z, T)} \right\} d\tau + f_C(x, y, z) +$$

$$\Omega \frac{\partial}{\partial x} \int_0^t \frac{D_S}{k T} \nabla_S \mu(x, y, z, \tau) \int_0^{L_z} [\alpha_{2C} + C_1(x, y, W, \tau)] dW d\tau + \frac{\partial}{\partial y} \int_0^t \nabla_S \mu(x, y, z, \tau) \times$$

$$\Omega \frac{D_S}{k T} \int_0^{L_z} [\alpha_{2C} + C_1(x, y, W, \tau)] dW d\tau + \frac{\partial}{\partial x} \left[ \frac{D_{CS}}{\bar{V} k T} \frac{\partial \mu_2(x, y, z, t)}{\partial x} \right] +$$

$$\frac{\partial}{\partial y} \left[ \frac{D_{CS}}{\bar{V} k T} \frac{\partial \mu_2(x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[ \frac{D_{CS}}{\bar{V} k T} \frac{\partial \mu_2(x, y, z, t)}{\partial z} \right] \tag{1e}$$

$$I_2(x, y, z, t) = \frac{\partial}{\partial x} \int_0^t D_I(x, y, z, T) \frac{\partial I_1(x, y, z, \tau)}{\partial x} d\tau + \frac{\partial}{\partial y} \int_0^t D_I(x, y, z, T) \frac{\partial I_1(x, y, z, \tau)}{\partial y} d\tau +$$

$$\frac{\partial}{\partial z} \int_0^t D_I(x, y, z, T) \frac{\partial I_1(x, y, z, \tau)}{\partial z} d\tau - \int_0^t k_{I,I}(x, y, z, T) [\alpha_{2I} + I_1(x, y, z, \tau)]^2 d\tau -$$

$$\int_0^t k_{I,V}(x, y, z, T) [\alpha_{2I} + I_1(x, y, z, \tau)] [\alpha_{2V} + V_1(x, y, z, \tau)] d\tau + \frac{\partial}{\partial x} \int_0^t \nabla_S \mu(x, y, z, \tau) \times$$

$$\Omega \frac{D_{IS}}{k T} \int_0^{L_z} [\alpha_{2I} + I_1(x, y, W, \tau)] dW d\tau + \frac{\partial}{\partial y} \int_0^t \nabla_S \mu(x, y, z, \tau) \int_0^{L_z} [\alpha_{2I} + I_1(x, y, W, \tau)] \times$$

$$\Omega \frac{D_{IS}}{kT} dW d\tau + \frac{\partial}{\partial x} \left[ \frac{D_{IS}}{\bar{V}kT} \frac{\partial \mu_2(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ \frac{D_{IS}}{\bar{V}kT} \frac{\partial \mu_2(x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[ \frac{D_{IS}}{\bar{V}kT} \frac{\partial \mu_2(x, y, z, t)}{\partial z} \right] + f_I(x, y, z) \tag{3e}$$

$$V_2(x, y, z, t) = \frac{\partial}{\partial x} \int_0^t D_V(x, y, z, T) \frac{\partial V_1(x, y, z, \tau)}{\partial x} d\tau + \frac{\partial}{\partial y} \int_0^t D_V(x, y, z, T) \frac{\partial V_1(x, y, z, \tau)}{\partial y} d\tau +$$

$$\frac{\partial}{\partial z} \int_0^t D_V(x, y, z, T) \frac{\partial V_1(x, y, z, \tau)}{\partial z} d\tau - \int_0^t k_{V,V}(x, y, z, T) [\alpha_{2V} + V_1(x, y, z, \tau)]^2 d\tau -$$

$$\int_0^t k_{I,V}(x, y, z, T) [\alpha_{2I} + I_1(x, y, z, \tau)] [\alpha_{2V} + V_1(x, y, z, \tau)] d\tau + \frac{\partial}{\partial x} \int_0^t \nabla_S \mu(x, y, z, \tau) \times$$

$$\Omega \frac{D_{VS}}{kT} \int_0^{L_z} [\alpha_{2V} + V_1(x, y, W, \tau)] dW d\tau + \frac{\partial}{\partial y} \int_0^t \nabla_S \mu(x, y, z, \tau) \int_0^{L_z} [\alpha_{2V} + V_1(x, y, W, \tau)] \times$$

$$\Omega \frac{D_{VS}}{kT} dW d\tau + \frac{\partial}{\partial x} \left[ \frac{D_{VS}}{\bar{V}kT} \frac{\partial \mu_2(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[ \frac{D_{VS}}{\bar{V}kT} \frac{\partial \mu_2(x, y, z, t)}{\partial y} \right] +$$

$$\frac{\partial}{\partial z} \left[ \frac{D_{VS}}{\bar{V}kT} \frac{\partial \mu_2(x, y, z, t)}{\partial z} \right] + f_V(x, y, z)$$

$$\Phi_{2I}(x, y, z, t) = \frac{\partial}{\partial x} \int_0^t D_{\Phi_I}(x, y, z, T) \frac{\partial \Phi_{1I}(x, y, z, \tau)}{\partial x} d\tau + \frac{\partial}{\partial y} \int_0^t \frac{\partial \Phi_{1I}(x, y, z, \tau)}{\partial y} \times$$

$$D_{\Phi_I}(x, y, z, T) d\tau + \frac{\partial}{\partial z} \int_0^t D_{\Phi_I}(x, y, z, T) \frac{\partial \Phi_{1I}(x, y, z, \tau)}{\partial z} d\tau + \Omega \frac{\partial}{\partial x} \int_0^t \nabla_S \mu(x, y, z, \tau) \times$$

$$\frac{D_{\Phi_I}}{kT} \int_0^{L_z} [\alpha_{2\Phi_I} + \Phi_{1I}(x, y, W, \tau)] dW d\tau + \Omega \frac{\partial}{\partial y} \int_0^t \frac{D_{\Phi_I}}{kT} \int_0^{L_z} [\alpha_{2\Phi_I} + \Phi_{1I}(x, y, W, \tau)] dW \times$$

$$\nabla_S \mu(x, y, z, \tau) d\tau + \int_0^t k_{I,I}(x, y, z, T) I^2(x, y, z, \tau) d\tau + \frac{\partial}{\partial x} \int_0^t \frac{D_{\Phi_I}}{\bar{V}kT} \frac{\partial \mu_2(x, y, z, \tau)}{\partial x} d\tau +$$

$$\frac{\partial}{\partial y} \int_0^t \frac{D_{\Phi_I}}{\bar{V}kT} \frac{\partial \mu_2(x, y, z, \tau)}{\partial y} d\tau + \frac{\partial}{\partial z} \int_0^t \frac{D_{\Phi_I}}{\bar{V}kT} \frac{\partial \mu_2(x, y, z, \tau)}{\partial z} d\tau + f_{\Phi_I}(x, y, z) +$$

$$\int_0^t k_I(x, y, z, T) I(x, y, z, \tau) d\tau \tag{5e}$$



$$\begin{aligned} \Phi_{2V}(x, y, z, t) &= \frac{\partial}{\partial x} \int_0^t D_{\Phi_V}(x, y, z, T) \frac{\partial \Phi_{1V}(x, y, z, \tau)}{\partial x} d\tau + \frac{\partial}{\partial y} \int_0^t \frac{\partial \Phi_{1V}(x, y, z, \tau)}{\partial y} \times \\ &D_{\Phi_V}(x, y, z, T) d\tau + \frac{\partial}{\partial z} \int_0^t D_{\Phi_V}(x, y, z, T) \frac{\partial \Phi_{1V}(x, y, z, \tau)}{\partial z} d\tau + \Omega \frac{\partial}{\partial x} \int_0^t \nabla_S \mu(x, y, z, \tau) \times \\ &\frac{D_{\Phi_{rS}}}{kT} \int_0^{L_z} [\alpha_{2\Phi_V} + \Phi_{1V}(x, y, W, \tau)] dW d\tau + \Omega \frac{\partial}{\partial y} \int_0^t \frac{D_{\Phi_{rS}}}{kT} \int_0^{L_z} [\alpha_{2\Phi_V} + \Phi_{1V}(x, y, W, \tau)] dW \times \\ &\nabla_S \mu(x, y, z, \tau) d\tau + \int_0^t k_{V,V}(x, y, z, T) V^2(x, y, z, \tau) d\tau + \frac{\partial}{\partial x} \int_0^t \frac{D_{\Phi_{rS}}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, \tau)}{\partial x} d\tau + \\ &\frac{\partial}{\partial y} \int_0^t \frac{D_{\Phi_{rS}}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, \tau)}{\partial y} d\tau + \frac{\partial}{\partial z} \int_0^t \frac{D_{\Phi_{rS}}}{\bar{V} kT} \frac{\partial \mu_2(x, y, z, \tau)}{\partial z} d\tau + f_{\Phi_V}(x, y, z) + \\ &\int_0^t k_V(x, y, z, T) V(x, y, z, \tau) d\tau. \end{aligned}$$

The next standard relation gives a possibility to calculate average values of the second-order approximations of the above concentrations.<sup>[28]</sup>

$$\alpha_{2\rho} = \frac{1}{\Theta L_x L_y L_z} \int_0^{\Theta} \int_0^{L_x} \int_0^{L_y} \int_0^{L_z} [\rho_2(x, y, z, t) - \rho_1(x, y, z, t)] dz dy dx dt \quad (10)$$

Substitution of the second-order approximations of the considered concentrations into relation Eqs. (10) gives a possibility to obtain relations for required average values  $\alpha_{2r}$

$$\begin{aligned} \alpha_{2C} = 0, \alpha_{2FI} = 0, \alpha_{2FV} = 0, \alpha_{2V} &= \sqrt{\frac{(b_3 + E)^2}{4b_4^2} - 4 \left( F + \frac{\Theta a_3 F + \Theta^2 L_x L_y L_z b_1}{b_4} \right)} - \frac{b_3 + E}{4b_4}, \\ \alpha_{2I} &= \frac{C_V - \alpha_{2V}^2 S_{VV00} - \alpha_{2V} (2S_{VV01} + S_{IV10} + \Theta L_x L_y L_z) - S_{VV02} - S_{IV11}}{S_{IV01} + \alpha_{2V} S_{IV00}}. \end{aligned}$$

$$\begin{aligned} \text{Here } b_4 &= \frac{1}{\Theta L_x L_y L_z} S_{IV00}^2 S_{VV00} - \frac{1}{\Theta L_x L_y L_z} S_{VV00}^2 S_{II00}, b_3 = -\frac{S_{II00} S_{VV00}}{\Theta L_x L_y L_z} (2S_{VV01} + S_{IV10} + \\ &\Theta L_x L_y L_z) + \frac{S_{IV00} S_{VV00}}{\Theta L_x L_y L_z} (S_{IV01} + 2S_{II10} + S_{IV01} + \Theta L_x L_y L_z) + \frac{S_{IV00}^2}{\Theta L_x L_y L_z} (2S_{VV01} + S_{IV10} + \\ &\Theta L_x L_y L_z) - \frac{S_{IV00}^2 S_{IV10}}{\Theta^3 L_x^3 L_y^3 L_z^3}, b_2 = \frac{S_{II00} S_{VV00}}{\Theta L_x L_y L_z} (S_{VV02} + S_{IV11} + C_V) - (S_{IV10} - 2S_{VV01} + \Theta L_x L_y \times \\ &L_z)^2 + \frac{S_{IV01} S_{VV00}}{\Theta L_x L_y L_z} (\Theta L_x L_y L_z + 2S_{II10} + S_{IV01}) + \frac{S_{IV00}}{\Theta L_x L_y L_z} (S_{IV01} + 2S_{II10} + 2S_{IV01} + \Theta L_x L_y \times \\ &L_z) (2S_{VV01} + \Theta L_x L_y L_z + S_{IV10}) - \frac{S_{IV00}^2}{\Theta L_x L_y L_z} (C_V - S_{VV02} - S_{IV11}) + \frac{C_V S_{IV00}^2}{\Theta^2 L_x^2 L_y^2 L_z^2} - \frac{2S_{IV10}}{\Theta L_x L_y L_z} \times \end{aligned}$$

$$S_{IV00}S_{IV01}, b_1 = S_{II00} \frac{S_{IV11} + S_{VV02} + C_V}{\Theta L_x L_y L_z} (2S_{VV01} + S_{IV10} + \Theta L_x L_y L_z) + \frac{S_{IV01}}{\Theta L_x L_y L_z} (\Theta L_x L_y \times$$

$$L_z + 2S_{II10} + S_{IV01}) (2S_{VV01} + S_{IV10} + \Theta L_x L_y L_z) - \frac{S_{IV10} S_{IV01}^2}{\Theta L_x L_y L_z} - \frac{S_{IV00}}{\Theta L_x L_y L_z} (3S_{IV01} + 2S_{II10} +$$

$$\Theta L_x L_y L_z) (C_V - S_{VV02} - S_{IV11}) + 2C_I S_{IV00} S_{IV01}, b_0 = \frac{S_{II00}}{\Theta L_x L_y L_z} (S_{IV00} + S_{VV02})^2 - \frac{S_{IV01}}{L_x L_y L_z} \times$$

$$\frac{1}{\Theta} (\Theta L_x L_y L_z + 2S_{II10} + S_{IV01}) (C_V - S_{VV02} - S_{IV11}) + 2C_I S_{IV01}^2 - S_{IV01} \frac{C_V - S_{VV02} - S_{IV11}}{\Theta L_x L_y L_z} \times$$

$$\frac{1}{\Theta} (\Theta L_x L_y L_z + 2S_{II10} + S_{IV01}) (C_V - S_{VV02} - S_{IV11}) + 2C_I S_{IV01}^2 -$$

$$S_{IV01} \frac{C_V - S_{VV02} - S_{IV11}}{\Theta L_x L_y L_z} \times (\Theta L_x L_y L_z + 2S_{II10} + S_{IV01}),$$

$$C_I = \frac{\alpha_{1I} \alpha_{1V}}{\Theta L_x L_y L_z} S_{IV00} + \frac{\alpha_{1I}^2 S_{II00}}{\Theta L_x L_y L_z} - \frac{S_{II20} S_{II20}}{\Theta L_x L_y L_z} - \frac{S_{IV11}}{\Theta L_x L_y L_z},$$

$$C_V = \alpha_{1I} \alpha_{1V} S_{IV00} + \alpha_{1V}^2 S_{VV00} - S_{VV02} - S_{IV11}, E = \sqrt{8y + \Theta^2 \frac{a_3^2}{a_4^2} - 4\Theta \frac{a_2}{a_4}}, F = \frac{\Theta a_2}{6a_4} +$$

$$\sqrt[3]{\sqrt{r^2 + s^3} - r} - \sqrt[3]{\sqrt{r^2 + s^3} + r}, r = \frac{\Theta^3 b_2}{24b_4^2} \left( 4b_0 - \Theta L_x L_y L_z \frac{b_1 b_3}{b_4} \right) - \frac{\Theta^3 b_2^3}{54b_4^3} - b_0 \frac{\Theta^2}{8b_4^2} \times$$

$$\left( 4\Theta b_2 - \Theta^2 \frac{b_3^2}{b_4} \right) - L_x^2 L_y^2 L_z^2 \frac{\Theta^4 b_1^2}{8b_4^2}, s = \Theta^2 \frac{4b_0 b_4 - \Theta L_x L_y L_z b_1 b_3}{12b_4^2} - \frac{\Theta b_2}{18b_4}.$$

Now, we calculate solutions of Eqs. (8) by the same method of averaging function corrections. Equations for the first-order approximations of the considered components could be written as

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

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

The solution of the above equations could be obtained by integration both their sides. Result of this integration takes the form

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

$$K(z) \frac{\beta(z)}{\rho(z)} \frac{\partial}{\partial x} \int_0^\infty \int_0^\vartheta T(x, y, z, \tau) d\tau d\vartheta.$$

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

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

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

$$K(z) \frac{\beta(z)}{\rho(z)} \frac{\partial}{\partial z} \int_0^\infty \int_0^\vartheta T(x, y, z, \tau) d\tau d\vartheta.$$

Equations for the second-order approximations of displacement vector components could be obtained framework standard procedure of the method of averaging of function corrections<sup>[28]</sup> and could be written as

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

$$\frac{\partial^2 u_{1y}(x, y, z, t)}{\partial x \partial y} + \frac{E(z)}{2[1+\sigma(z)]} \left[ \frac{\partial^2 u_{1y}(x, y, z, t)}{\partial y^2} + \frac{\partial^2 u_{1z}(x, y, z, t)}{\partial z^2} \right] - \frac{\partial T(x, y, z, t)}{\partial x} \times$$

$$K(z)\beta(z) + \left\{ K(z) + \frac{E(z)}{3[1+\sigma(z)]} \right\} \frac{\partial^2 u_{1z}(x, y, z, t)}{\partial x \partial z}$$

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

$$K(z)\beta(z) + \frac{\partial}{\partial z} \left\{ \frac{E(z)}{2[1+\sigma(z)]} \left[ \frac{\partial u_{1y}(x, y, z, t)}{\partial z} + \frac{\partial u_{1z}(x, y, z, t)}{\partial y} \right] \right\} + \frac{\partial^2 u_{1y}(x, y, z, t)}{\partial y^2} \times$$

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

$$\rho(z) \frac{\partial^2 u_{2z}(x, y, z, t)}{\partial t^2} = \frac{E(z)}{2[1+\sigma(z)]} \left[ \frac{\partial^2 u_{1z}(x, y, z, t)}{\partial x^2} + \frac{\partial^2 u_{1z}(x, y, z, t)}{\partial y^2} + \frac{\partial^2 u_{1x}(x, y, z, t)}{\partial x \partial z} +$$

$$\frac{\partial^2 u_{1y}(x, y, z, t)}{\partial y \partial z} \right] + \frac{\partial}{\partial z} \left\{ K(z) \left[ \frac{\partial u_{1x}(x, y, z, t)}{\partial x} + \frac{\partial u_{1y}(x, y, z, t)}{\partial y} + \frac{\partial u_{1x}(x, y, z, t)}{\partial z} \right] \right\} +$$

$$\frac{E(z)}{6[1+\sigma(z)]} \frac{\partial}{\partial z} \left[ 6 \frac{\partial u_{1z}(x, y, z, t)}{\partial z} - \frac{\partial u_{1x}(x, y, z, t)}{\partial x} - \frac{\partial u_{1y}(x, y, z, t)}{\partial y} - \frac{\partial u_{1z}(x, y, z, t)}{\partial z} \right] -$$

$$\left. \frac{\partial u_{1x}(x, y, z, t)}{\partial x} - \frac{\partial u_{1y}(x, y, z, t)}{\partial y} - \frac{\partial u_{1z}(x, y, z, t)}{\partial z} \right\} \frac{E(z)}{1 + \sigma(z)} - K(z) \beta(z) \frac{\partial T(x, y, z, t)}{\partial z}.$$

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

$$\begin{aligned} 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) - \right. \\ & \frac{E(z)}{3[1 + \sigma(z)]} \left. \right\} \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)}{2\rho(z)} \left[ \frac{\partial^2}{\partial y^2} \int_0^t \int_0^\vartheta u_{1y}(x, y, z, \tau) d\tau d\vartheta + \right. \\ & \left. \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}{1 + \sigma(z)} + \frac{1}{\rho(z)} \frac{\partial^2}{\partial x \partial z} \int_0^t \int_0^\vartheta u_{1z}(x, y, z, \tau) d\tau d\vartheta \left\{ K(z) + \right. \\ & \left. \frac{E(z)}{3[1 + \sigma(z)]} \right\} - 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 - \frac{\partial^2}{\partial x^2} \int_0^\infty \int_0^\vartheta u_{1x}(x, y, z, \tau) d\tau d\vartheta \times \\ & \frac{1}{\rho(z)} \left\{ K(z) + \frac{5E(z)}{6[1 + \sigma(z)]} \right\} - \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 \times \\ & \left. \frac{1}{\rho(z)} - \frac{E(z)}{2\rho(z)[1 + \sigma(z)]} \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] - \right. \\ & \left. \frac{1}{\rho(z)} \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 + u_{0x} + K(z) \frac{\beta(z)}{\rho(z)} \times \right. \\ & \left. \frac{\partial}{\partial x} \int_0^\infty \int_0^\vartheta T(x, y, z, \tau) d\tau d\vartheta \right. \\ 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{1}{1 + \sigma(z)} + \frac{K(z)}{\rho(z)} \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)} \left\{ \frac{5E(z)}{12[1 + \sigma(z)]} + K(z) \right\} \times \\ & \frac{\partial^2}{\partial y^2} \int_0^t \int_0^\vartheta u_{1x}(x, y, z, \tau) d\tau d\vartheta + \frac{1}{2\rho(z)} \frac{\partial}{\partial z} \left\{ \frac{E(z)}{1 + \sigma(z)} \left[ \frac{\partial}{\partial z} \int_0^t \int_0^\vartheta u_{1y}(x, y, z, \tau) d\tau d\vartheta + \right. \right. \\ & \left. \left. \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 - \left\{ \frac{E(z)}{6[1 + \sigma(z)]} - \right. \end{aligned}$$

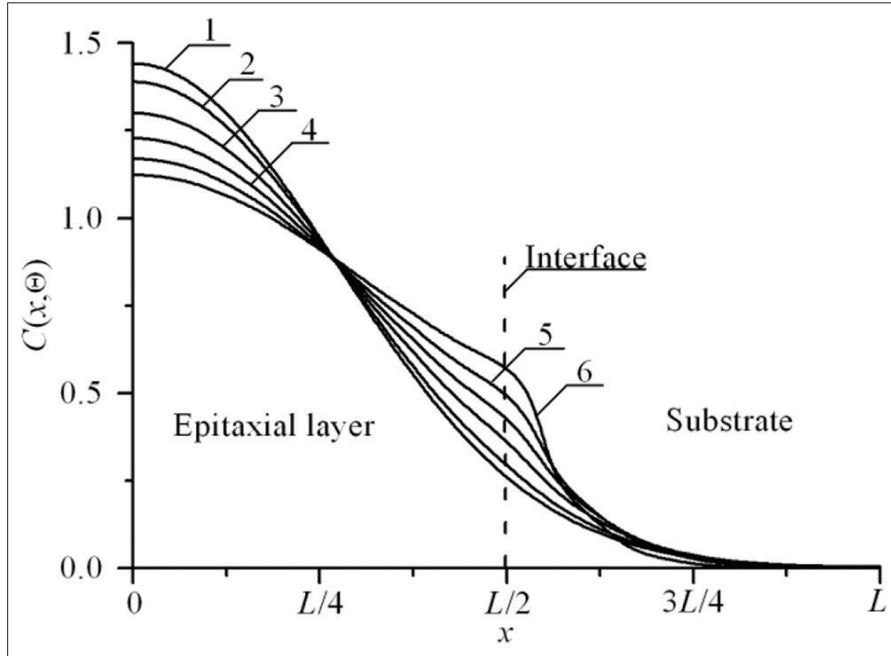
$$\begin{aligned}
 & -K(z)\left\{\frac{1}{\rho(z)}\frac{\partial^2}{\partial y\partial z}\int_0^\vartheta\int_0^\vartheta u_{1y}(x,y,z,\tau)d\tau d\vartheta - \frac{E(z)}{2\rho(z)}\left[\frac{\partial^2}{\partial x^2}\int_0^\vartheta\int_0^\vartheta u_{1x}(x,y,z,\tau)d\tau d\vartheta + \right. \right. \\
 & \left. \left. \frac{\partial^2}{\partial x\partial y}\int_0^\vartheta\int_0^\vartheta u_{1x}(x,y,z,\tau)d\tau d\vartheta\right]\frac{1}{1+\sigma(z)} - K(z)\frac{\beta(z)}{\rho(z)}\int_0^\vartheta\int_0^\vartheta T(x,y,z,\tau)d\tau d\vartheta - \frac{K(z)}{\rho(z)}\times \right. \\
 & \left. \frac{\partial^2}{\partial x\partial y}\int_0^\vartheta\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^\vartheta\int_0^\vartheta u_{1x}(x,y,z,\tau)d\tau d\vartheta\left\{\frac{5E(z)}{12[1+\sigma(z)]} + \right. \right. \\
 & \left. \left. K(z)\right\} - \frac{\partial}{\partial z}\left\{\frac{E(z)}{1+\sigma(z)}\left[\frac{\partial}{\partial z}\int_0^\vartheta\int_0^\vartheta u_{1y}(x,y,z,\tau)d\tau d\vartheta + \frac{\partial}{\partial y}\int_0^\vartheta\int_0^\vartheta u_{1z}(x,y,z,\tau)d\tau d\vartheta\right]\right\}\times \\
 & \left. \frac{1}{2\rho(z)} - \frac{1}{\rho(z)}\left\{K(z) - \frac{E(z)}{6[1+\sigma(z)]}\right\}\frac{\partial^2}{\partial y\partial z}\int_0^\vartheta\int_0^\vartheta u_{1y}(x,y,z,\tau)d\tau d\vartheta + u_{0y}, \right. \\
 & \left. u_z(x,y,z,t) = \frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial^2}{\partial x^2}\int_0^\vartheta\int_0^\vartheta u_{1z}(x,y,z,\tau)d\tau d\vartheta + \frac{\partial^2}{\partial y^2}\int_0^\vartheta\int_0^\vartheta u_{1z}(x,y,z,\tau)d\tau d\vartheta + \right. \right. \\
 & \left. \left. \frac{\partial^2}{\partial x\partial z}\int_0^\vartheta\int_0^\vartheta u_{1x}(x,y,z,\tau)d\tau d\vartheta + \frac{\partial^2}{\partial y\partial z}\int_0^\vartheta\int_0^\vartheta u_{1y}(x,y,z,\tau)d\tau d\vartheta\right]\frac{1}{\rho(z)} + \frac{1}{\rho(z)}\times \right. \\
 & \left. \frac{\partial}{\partial z}\left\{K(z)\left[\frac{\partial}{\partial x}\int_0^\vartheta\int_0^\vartheta u_{1x}(x,y,z,\tau)d\tau d\vartheta + \frac{\partial}{\partial y}\int_0^\vartheta\int_0^\vartheta u_{1x}(x,y,z,\tau)d\tau d\vartheta + \right. \right. \right. \\
 & \left. \left. \frac{\partial}{\partial z}\int_0^\vartheta\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^\vartheta\int_0^\vartheta u_{1z}(x,y,z,\tau)d\tau d\vartheta - \right. \right. \\
 & \left. \left. \frac{\partial}{\partial x}\int_0^\vartheta\int_0^\vartheta u_{1x}(x,y,z,\tau)d\tau d\vartheta - \frac{\partial}{\partial y}\int_0^\vartheta\int_0^\vartheta u_{1y}(x,y,z,\tau)d\tau d\vartheta - \frac{\partial}{\partial z}\int_0^\vartheta\int_0^\vartheta u_{1z}(x,y,z,\tau)d\tau d\vartheta\right]\right\} - \\
 & \left. K(z)\frac{\beta(z)}{\rho(z)}\frac{\partial}{\partial z}\int_0^\vartheta\int_0^\vartheta T(x,y,z,\tau)d\tau d\vartheta + u_{0z}. \right.
 \end{aligned}$$

In this paper, we calculate distributions of concentration of dopant and radiation defects in space and time using the second-order approximation framework method of averaging of function corrections. We also calculate distributions of components of displacement vector in space and time framework the same approximation. Usually, the second-order approximation is enough good approximation to obtain some quantitative results and to make the qualitative analysis. All obtained results have been checked by comparison with the results of numerical simulations.

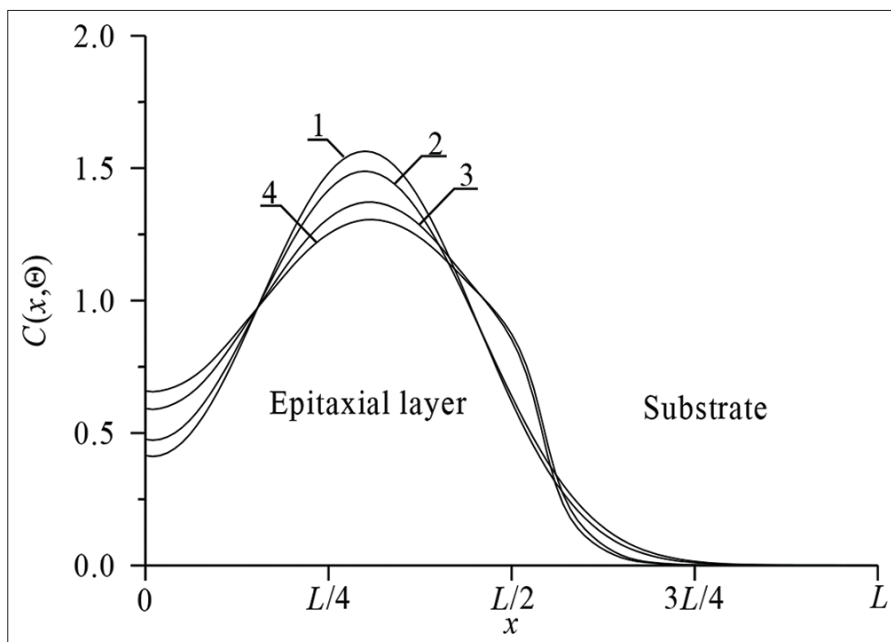
## DISCUSSION

Now, we will be analyzing the redistributions of radiation defects and dopant during annealing. In this situation, we take into account the influence of modification of porosity and mismatch-induced

stress on the redistribution of radiation defects and dopant. We present several spatial distributions of concentrations of dopant in heterostructures, as shown in Figures 2 and 3. Figure 2 corresponds to the diffusion type of doping. Figure 3 corresponds to ion type of doping. All distributions of dopant correspond to the larger value of dopant diffusion coefficient in comparison with the nearest areas. One can find that inhomogeneity of heterostructure leads to increasing homogeneity of dopant in the doped area of the epitaxial layer. However, it should be noted that optimization of annealing of dopant and/or radiation defects required to obtain a compromise between increasing of homogeneity of distribution of concentration of dopant in the required area and increasing.



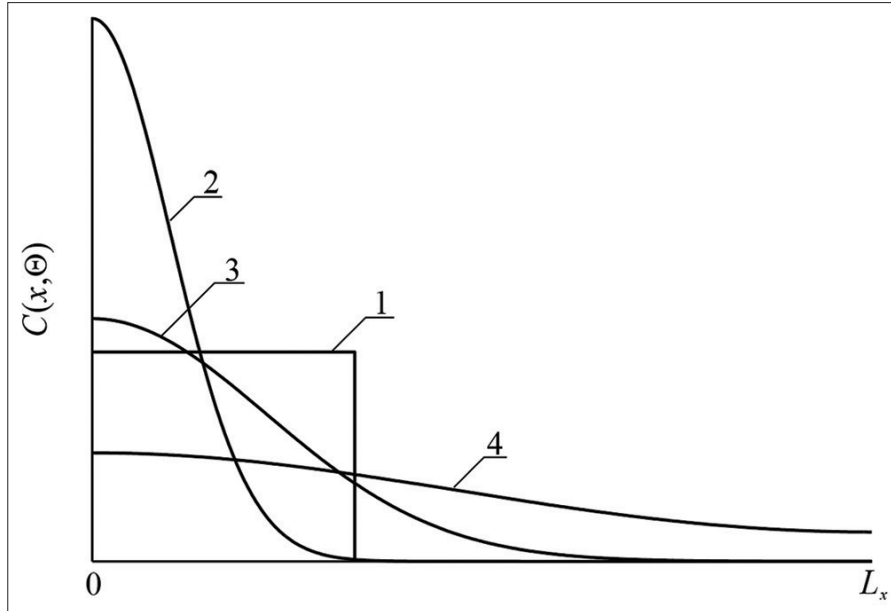
**Figure 2:** Spatial distributions of infused dopant concentration in the considered heterostructure in the perpendicular direction to interface between epitaxial layer and substrate. The larger number of curves corresponds to the larger difference between values of dopant diffusion coefficient in the heterostructure. Value of dopant diffusion coefficient in the substrate is smaller, than the value of dopant diffusion coefficient in the epitaxial layer



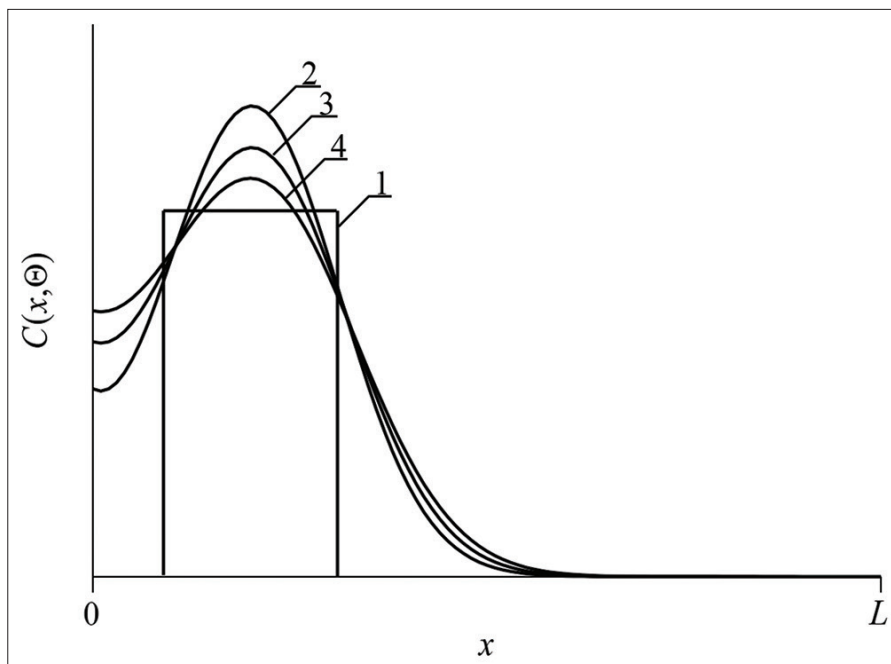
**Figure 3:** Spatial distributions of implanted dopant concentration in the considered heterostructure in the perpendicular direction to interface between epitaxial layer and substrate. Curves 1 and 3 were calculated for time of annealing  $\Theta = 0.0048(L_x^2 + L_y^2 + L_z^2)/D_0$ . Curves 2 and 4 were calculated for time of annealing  $\Theta = 0.0057(L_x^2 + L_y^2 + L_z^2)/D_0$ . Curves 1 and 2 were calculated for homogenous samples. Curves 3 and 4 were calculated for heterostructure for the case, when the diffusion coefficient of dopant in the substrate is smaller than the diffusion coefficient of dopant in the epitaxial layer

$$U = \frac{1}{L_x L_y L_z} \int_0^{L_x} \int_0^{L_y} \int_0^{L_z} [C(x, y, z, \Theta) - \psi(x, y, z)] dz dy dx \quad (15)$$

to determine the compromise value of annealing time. Here,  $\psi(x, y, z)$  is the considered step-wise approximation function [Figure 5]. Figures 6 (for diffusion type of doping) and 7 (for ion type of doping) show optimal annealing times as functions of several parameters. It is known that anneal radiation defects after ion implantation should be done. Spatial distributions of dopant will spread during this annealing.



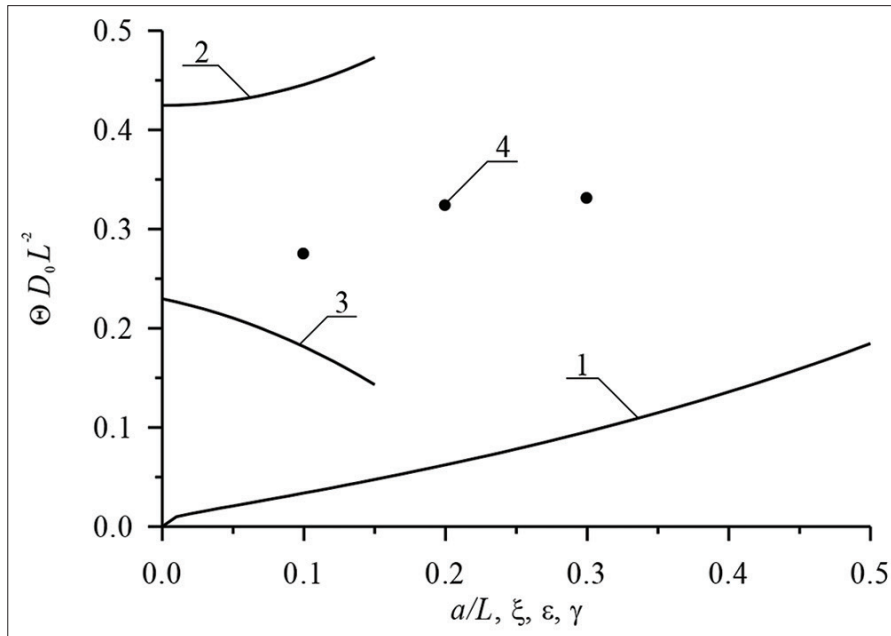
**Figure 4:** Spatial distributions of concentration of the infused dopant in the considered heterostructure. Curve 1 shows idealized dopant distribution (step-wise function). Curves 2–4 show real dopant distributions at the different continuance of annealing. The larger value of the number of curves mean larger value of continuance of annealing



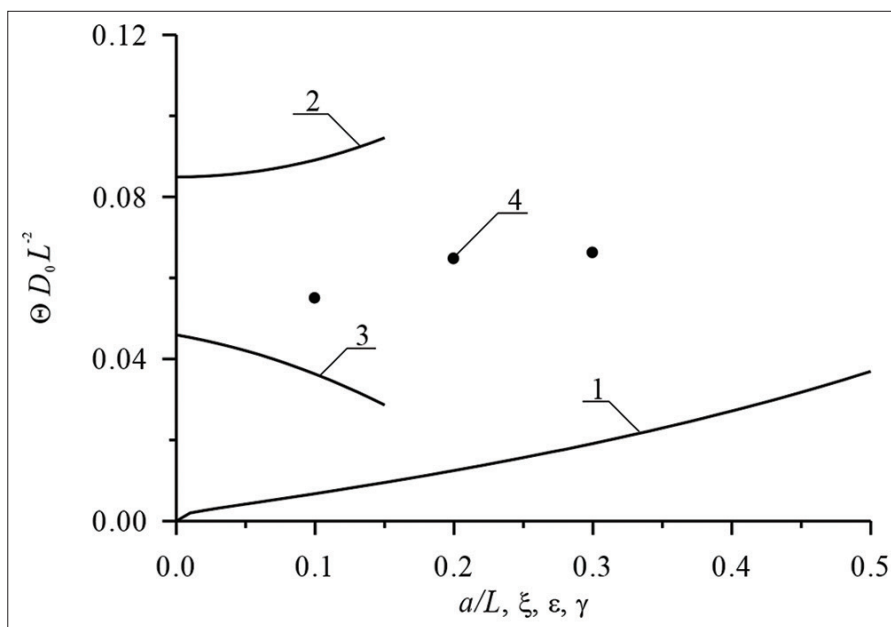
**Figure 5:** Spatial distributions of concentration of the implanted dopant in the considered heterostructure. Curve 1 shows idealized dopant distribution (step-wise function). Curves 2–4 show real dopant distributions at the different continuance of annealing. Larger value of the number of the curve means larger value of continuance of annealing sharpness of this distribution after this area. To obtain this compromise, we used recently introduced criterion.<sup>[29-37]</sup> To use this criterion, one shall approximate real spatial distribution of dopant concentration by required step-wise function (Figure 4 for diffusion type of doping and 5 for ion type of doping). After that, one shall minimize the mean-squared error

The dopant should achieve the required interface between layers of heterostructure during the annealing. If dopant cannot achieve during the radiation defects annealing, it is attracted an interest additional annealing of the dopant. In this situation, one can find the smaller value of implanted dopant annealing time in comparison with annealing time of infused dopant.

Now, we consider the influence of variation of miss-match induced stress on the dopant concentration distribution in the considered heterostructure. At  $e_0 < 0$ , a compression of dopant concentration distribution could be found near the interface between layers of the heterostructure. On the other hand (at  $e_0 > 0$ ), the spreading of the distribution could be found. The variation of distribution could be partially decreased by laser annealing<sup>[37]</sup> due to the acceleration of dopant diffusion during this procedure. Mismatch-

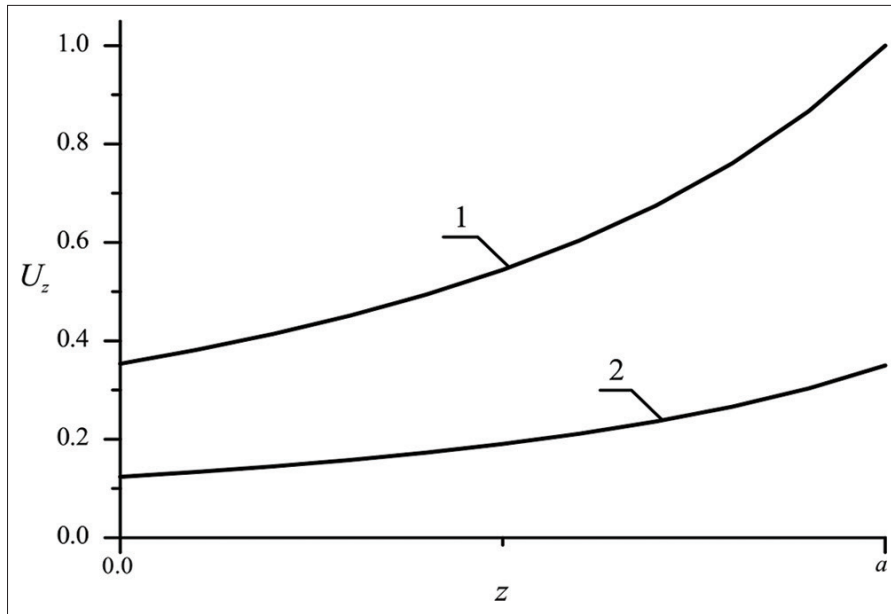


**Figure 6:** Dimensionless optimal annealing time of infused dopant as functions of several parameters. Curve 1 describes dependence of the annealing time on  $a/L$  at  $\xi = \gamma = 0$  in homogenous material. Curve 2 describes dependence of the annealing time on  $\epsilon$  at  $a/L=1/2$  and  $\xi = \gamma = 0$ . Curve 3 describes dependence of the annealing time on  $\xi$  at  $a/L=1/2$  and  $\epsilon = \gamma = 0$ . Curve 4 describes dependence of the annealing time on  $\gamma$  at  $a/L=1/2$  and  $\epsilon = \xi = 0$

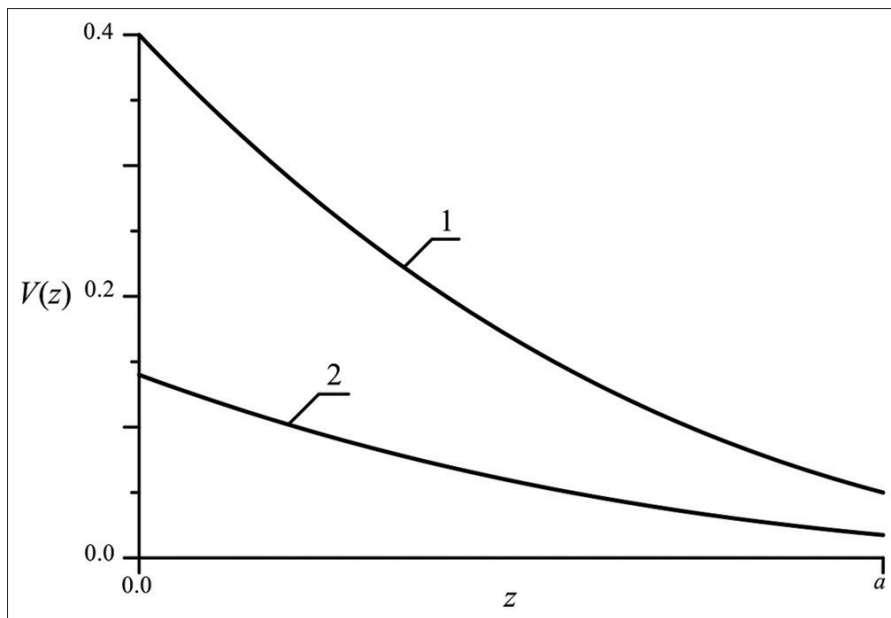


**Figure 7:** Dimensionless optimal annealing time of infused dopant as functions of several parameters. Curve 1 describes dependence of the annealing time on  $a/L$  at  $\xi = \gamma = 0$  in homogenous material. Curve 2 describes dependence of the annealing time on  $\epsilon$  at  $a/L=1/2$  and  $\xi = \gamma = 0$ . Curve 3 describes dependence of the annealing time on  $\xi$  at  $a/L=1/2$  and  $\epsilon = \gamma = 0$ . Curve 4 describes dependence of the annealing time on  $\gamma$  at  $a/L=1/2$  and  $\epsilon = \xi = 0$





**Figure 8:** Dependences of the normalized component of displacement vector on coordinate, which is perpendicular to the interface between layers of the heterostructure. Curve 1 corresponds to nonporous material. Curve 2 corresponds to porous material



**Figure 9:** Dependences of normalized vacancy concentrations on coordinate, which is perpendicular to the interface between layers of the heterostructure. Curve 1 corresponds to nonporous material. Curve 2 corresponds to porous material

induced stress in heterostructure leads to changing of value of optimal annealing time. At the same time, modification of porosity leads to decrease the value of mechanical stress. On the one hand, mismatch-induced stress could be used to increase the density of elements of integrated circuits. At the same time, the stress could leads to generation dislocations of the discrepancy. Figures 8 and 9 show vacancies concentration distributions in porous materials and component of the displacement vector, which are perpendicular to the interface between layers of the heterostructure.

## CONCLUSION

We analyzed the redistribution of implanted and infused dopants in a heterostructure with porous layer to manufacturing field-effect heterotransistors framework in a sense-amplifier based flip-flop. We also

analyzed the influence of relaxation mismatch-induced stress on the above redistribution. We obtain several recommendations to optimize annealing for decreasing dimensions of transistors and to increase their density framework integrated circuits. We also formulate conditions for decreasing mismatch-induced stress. An analytical approach to solve considered boundary problems with account nonlinearity of processes and changing of parameters in space and time has been introduced.

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