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On approach to decrease dimensions of element "OR" manufactured by using field-effect heterotransistor

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ABSTRACT

In this paper we introduce an approach to decrease dimensions of logical elements "OR" based on field-effect heterotransistor. The approach based on manufacture the heterostructure with required configuration, diffusion or ion doping of required areas of the heterostructure and optimization of annealing of dopant and/or radiation defects. Several recommendations to optimize annealing both dopant and radiation defects have been formulated.

INTRODUCTION

Development of solid state electronic leads to necessity to elaborate new electronic devices and to optimize existing one. One way of development of solid state electronic is increasing of density of elements of integrated circuits. Increasing of density of elements of integrated circuits leads to necessity to decrease dimensions of these elements[1-5]. The second way of development of solid state electronic is increasing of their performance[6-8]. The third way of the development is improve the material properties of electronic materials[9-11].

Let us consider logical element "OR" based on field-effect transistors, which was considered in Ref.[12] (see Figure 1). Framework our paper we introduce the approach to decrease dimensions of the logical element. The approach based on manufacturing a heterostructure with two layers: a substrate and an epitaxial layer (see Figure 1). The epitaxial layer should include into itself several sections manufactured by using another materials (see Figure 1). These sections have been doped by diffusion or ion implantation to generation required type of conductivity (n or p). Farther we consider annealing of dopant and/or radiation defects. It have been formulated recommendations for optimization annealing of dopant and/or radiation defects to manufacture more compact logical elements with higher homogeneity of distribution of concentration of dopant.

Method of solution

We determine spatio-temporal distribution of concentration of dopant by solving the following boundary problem

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

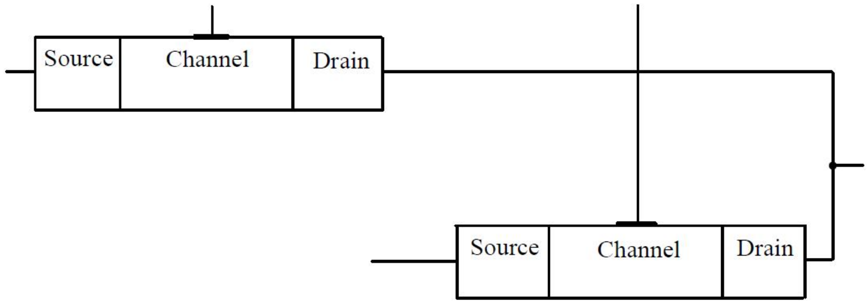

Figure 1a : Structure of element “OR”. View from top

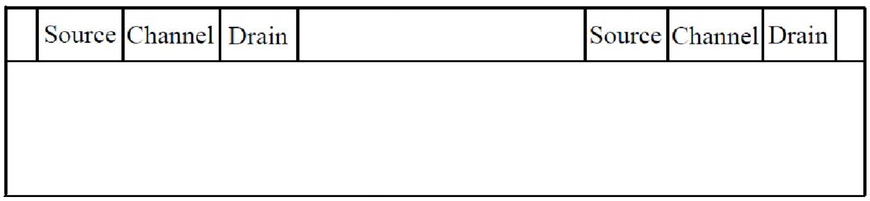

Figure 1b : Heterostructure with two layers and sections in the epitaxial layer. View from side

with boundary and initial conditions

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

$$\left.\frac{\partial C(x,y,z,t)}{\partial z}\right|_{z=0}=0,\ \left.\frac{\partial C(x,y,z,t)}{\partial z}\right|_{x=L_z}=0,\ C(x,y,z,0)=f(x,y,z). \qquad (2)$$

Here C(x,y,z,t) is the spatio-temporal distribution of concentration of dopant; T is the temperature of annealing; D_C is the dopant diffusion coefficient. Value of dopant diffusion coefficient depends on properties of materials of heterostructure, speed of heating and cooling of heterostructure (with account Arrhenius law). Dependences of dopant diffusion coefficient on parameters could be approximated by the following relation[13-15]

$$D_C=D_L(x,y,z,T)\left[1+\xi\frac{C^{\gamma}(x,y,z,t)}{P^{\gamma}(x,y,z,T)}\right]\left[1+\varsigma_1\frac{V(x,y,z,t)}{V^*}+\varsigma_2\frac{V^2(x,y,z,t)}{(V^*)^2}\right], \qquad (3)$$

where D_L (x,y,z,T) is the spatial (due to presents several layers in heterostructure) and temperature (due to Arrhenius law) dependences of dopant diffusion coefficient; P (x, y,z,T) is the limit of solubility of dopant; parameter γ depends on properties of materials and could be integer in the following interval $\gamma \in [1,3]$ [13]; V (x,y,z,t) is the spatio-temporal distribution of concentration of radiation vacancies; V^* is the equilibrium distribution of concentration of vacancies. Concentrational dependence of dopant diffusion coefficient has been described in details in[13]. Using diffusion type of doping did not generation radiation defects. In this situation $\zeta_1=\zeta_2= 0$. We determine the spatio-temporal distributions of concentrations of radiation defects by solving the following system of equations[14,15]

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

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

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$$-k_{I,I}(x,y,z,T)I^2(x,y,z,t) \quad (4)$$

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

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

$$-k_{V,V}(x,y,z,T)V^2(x,y,z,t)$$

with boundary and initial conditions

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

$$\left.\frac{\partial \rho(x,y,z,t)}{\partial z}\right|_{z=0}=0,\ \left.\frac{\partial \rho(x,y,z,t)}{\partial z}\right|_{z=L_z}=0,\ \rho(x,y,z,0)=f_\rho(x,y,z). \quad (5)$$

Here ρ =I,V; I (x,y,z,t) is the spatio-temporal distribution of concentration of radiation interstitials; D_ρ(x,y,z,T) are the diffusion coefficients of point radiation defects; terms V^2(x,y,z,t) and I^2(x,y,z,t) correspond to generation divacancies and diinterstitials; $k_{I,V}$(x,y,z,T) is the parameter of recombination of point radiation defects; $k_{I,I}$(x,y,z,T) and $k_{V,V}$(x,y,z,T) are the parameters of generation of simplest complexes of point radiation defects.

We determine the spatio-temporal distributions of concentrations of divacancies Φ_V (x,y,z,t) and dinterstitials Φ_I (x,y,z,t) by solving the following system of equations[14,15]

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

$$+\frac{\partial}{\partial z}\left[D_{\Phi I}(x,y,z,T)\frac{\partial \Phi_I(x,y,z,t)}{\partial z}\right]+k_{I,I}(x,y,z,T)I^2(x,y,z,t)-k_I(x,y,z,T)I(x,y,z,t) \quad (6)$$

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

$$+\frac{\partial}{\partial z}\left[D_{\Phi V}(x,y,z,T)\frac{\partial \Phi_V(x,y,z,t)}{\partial z}\right]+k_{V,V}(x,y,z,T)V^2(x,y,z,t)-k_V(x,y,z,T)V(x,y,z,t)$$

with boundary and initial conditions

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

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

$\Phi_I(x,y,z,0)=f_{\Phi I}(x,y,z)$, $\Phi_V(x,y,z,0)=f_{\Phi V}(x,y,z)$. **(7)**

Here $D_{\Phi\rho}(x,y,z,T)$ are the diffusion coefficients of the above complexes of radiation defects; $k_I(x,y,z,T)$ and $k_V(x,y,z,T)$ are the parameters of decay of these complexes.

To determine spatio-temporal distribution of concentration of dopant we transform the Eq.(1) to the following integro-differential form

$$\frac{xyz}{L_xL_yL_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}C(u,v,w,t)\,dw\,dv\,du=\frac{yz}{L_yL_z}\int_0^t\int_{L_y}^{y}\int_{L_z}^{z}\left[1+\varsigma_1\frac{V(x,v,w,\tau)}{V^*}+\varsigma_2\frac{V^2(x,v,w,\tau)}{(V^*)^2}\right]\times$$

$$\times D_L(x,v,w,T)\left[1+\xi\frac{C^\gamma(x,v,w,\tau)}{P^\gamma(x,v,w,T)}\right]\frac{\partial C(x,v,w,\tau)}{\partial x}\,d\tau+\frac{xz}{L_xL_z}\int_0^t\int_{L_x}^{x}\int_{L_z}^{z}D_L(u,y,w,T)\times$$

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

$$+\frac{xy}{L_xL_y}\int_0^t\int_{L_x}^{x}\int_{L_y}^{y}D_L(u,v,z,T)\left[1+\varsigma_1\frac{V(u,v,z,\tau)}{V^*}+\varsigma_2\frac{V^2(u,v,z,\tau)}{(V^*)^2}\right]\left[1+\xi\frac{C^\gamma(u,v,z,\tau)}{P^\gamma(x,y,z,T)}\right]\times$$

$$\times\frac{\partial C(u,v,z,\tau)}{\partial z}\,d\tau+\frac{xyz}{L_xL_yL_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}f(u,v,w)\,dw\,dv\,du. \quad \textbf{(1a)}$$

We determine solution of the above equation by using Bubnov-Galerkin approach[16]. Framework the approach we determine solution of the Eq.(1a) as the following series

$$C_0(x,y,z,t)=\sum_{n=1}^{N}a_{nC}\,c_n(x)\,c_n(y)\,c_n(z)\,e_{nC}(t),$$

where $e_{nC}(t)=\exp\left[-\pi^2n^2D_{0C}t\left(L_x^{-2}+L_y^{-2}+L_z^{-2}\right)\right]$, $c_n(\chi)=\cos(\pi n\chi/L_\chi)$. The above series includes into itself finite number of terms N. The considered series is similar with solution of linear Eq.(1) (i.e. with $\xi=0$) and averaged dopant diffusion coefficient D_0. Substitution of the series into Eq.(1a) leads to the following result

$$\frac{xyz}{\pi^2}\sum_{n=1}^{N}\frac{a_C}{n^3}s_n(x)\,s_n(y)\,s_n(z)\,e_{nC}(t)=-\frac{yz}{L_yL_z}\int_0^t\int_{L_y}^{y}\int_{L_z}^{z}\left\{1+\left[\sum_{n=1}^{N}a_{nC}\,c_n(x)\,c_n(v)\,c_n(w)\,e_{nC}(\tau)\right]^\gamma\times\right.$$

$$\left.\times\frac{\xi}{P^\gamma(x,v,w,T)}\right\}\left[1+\varsigma_1\frac{V(x,v,w,\tau)}{V^*}+\varsigma_2\frac{V^2(x,v,w,\tau)}{(V^*)^2}\right]D_L(x,v,w,T)\sum_{n=1}^{N}a_{nC}\,s_n(x)\,c_n(v)\times$$

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$$\times n\, c_n(w)\, e_{nC}(\tau) d\,\tau - \frac{x\,z}{L_x L_z} \int_0^t \int_{L_x}^x \int_{L_z}^z \left\{1 + \left[\sum_{m=1}^N a_{mC}\, c_m(u)\, c_m(y)\, c_m(w)\, e_{mC}(\tau)\right]^\gamma \frac{\xi}{P^\gamma(u,y,w,T)}\right\} \times$$

$$\times D_L(u,y,w,T)\left[1 + \varsigma_1 \frac{V(u,y,w,\tau)}{V^*} + \varsigma_2 \frac{V^2(u,y,w,\tau)}{(V^*)^2}\right] \sum_{n=1}^N n\, c_n(u)\, s_n(y)\, c_n(w)\, e_{nC}(\tau)\, d\,\tau \times$$

$$\times a_{nC} - \frac{x\,y}{L_x L_y} \int_0^t \int_{L_x}^x \int_{L_y}^y D_L(u,v,z,T) \left\{1 + \frac{\xi}{P^\gamma(u,v,z,T)} \left[\sum_{n=1}^N a_{nC}\, c_n(u)\, c_n(v)\, c_n(z)\, e_{nC}(\tau)\right]^\gamma\right\} \times$$

$$\times \left[1 + \varsigma_1 \frac{V(u,v,z,\tau)}{V^*} + \varsigma_2 \frac{V^2(u,v,z,\tau)}{(V^*)^2}\right] \sum_{n=1}^N n\, a_{nC} c_n(u)\, c_n(v)\, s_n(z)\, e_{nC}(\tau)\, d\,\tau + \frac{x\,y\,z}{L_x L_y L_z} \times$$

$$\times \int_{L_x}^x \int_{L_y}^y \int_{L_z}^z f(u,v,w)\, d\,w\, d\,v\, d\,u\,,$$

where $s_n(\chi) = \sin(\pi\, n\, \chi/L_\chi)$. We determine coefficients a_n by using orthogonality condition of terms of the considered series framework scale of heterostructure. The condition gives us possibility to obtain relations for calculation of parameters a_n for any quantity of terms N. In the common case the relations could be written as

$$-\frac{L_x^2 L_y^2 L_z^2}{\pi^5} \sum_{n=1}^N \frac{a_{nC}}{n^6} e_{nC}(t) = -\frac{L_y L_z}{2\pi^2} \int_0^t \int_0^{L_x} \int_0^{L_y} \int_0^{L_z} D_L(x,y,z,T) \left\{1 + \left[\sum_{n=1}^N a_{nC}\, c_n(x)\, c_n(y)\, c_n(z)\, e_{nC}(\tau)\right]^\gamma \times\right.$$

$$\left.\times \frac{\xi}{P^\gamma(x,y,z,T)}\right\} \left[1 + \varsigma_1 \frac{V(x,y,z,\tau)}{V^*} + \varsigma_2 \frac{V^2(x,y,z,\tau)}{(V^*)^2}\right] \sum_{n=1}^N \frac{a_{nC}}{n} s_n(2x)\, c_n(y)\, c_n(z)\, e_{nC}(\tau) \times$$

$$\times \left\{y\, s_n(y) + \frac{L_y}{\pi\, n}[c_n(y) - 1]\right\} \left\{z\, s_n(z) + \frac{L_z}{\pi\, n}[c_n(z) - 1]\right\} d\,z\, d\,y\, d\,x\, d\,\tau - \int_0^t \int_0^{L_x} \int_0^{L_y} \int_0^{L_z} D_L(x,y,z,T) \times$$

$$\times D_L(x,y,z,T) \left\{1 + \left[\sum_{n=1}^N a_{nC}\, c_n(x)\, c_n(y)\, c_n(z)\, e_{nC}(\tau)\right]^\gamma \frac{\xi}{P^\gamma(x,y,z,T)}\right\} \left[1 + \varsigma_1 \frac{V(x,y,z,\tau)}{V^*} + \right.$$

$$\left. + \varsigma_2 \frac{V^2(x,y,z,\tau)}{(V^*)^2}\right] \left[1 + \varsigma_1 \frac{V(x,y,z,\tau)}{V^*} + \varsigma_2 \frac{V^2(x,y,z,\tau)}{(V^*)^2}\right] \sum_{n=1}^N \left\{x\, s_n(x) + \frac{L_x}{\pi\, n}[c_n(x) - 1]\right\} \frac{a_{nC}}{n} \times$$

$$\times \frac{L_x L_z}{2\pi^2} c_n(x) s_n(2y)\, c_n(z)\, e_{nC}(\tau) \left\{z\, s_n(z) + \frac{L_z}{\pi\, n}[c_n(z) - 1]\right\} d\,z\, d\,y\, d\,x\, d\,\tau - \frac{L_x L_y}{2\pi^2} \times$$

$$\times \int_0^t \int_0^{L_x} \int_0^{L_y} \int_0^{L_z} \left\{1 + \left[\sum_{n=1}^N a_{nC}\, c_n(x)\, c_n(y)\, c_n(z)\, e_{nC}(\tau)\right]^\gamma \frac{\xi}{P^\gamma(x,y,z,T)}\right\} \left[1 + \varsigma_2 \frac{V^2(x,y,z,\tau)}{(V^*)^2} + \right.$$

$$+\varsigma_1\frac{V(x,y,z,\tau)}{V^*}\Bigg]D_L(x,y,z,T)\sum_{n=1}^{N}\frac{a_{nC}}{n}c_n(x)\,c_n(y)\,s_n(z)\left\{x\,s_n(x)+\frac{L_x}{\pi n}[c_n(x)-1]\right\}\times$$

$$\times\left\{y\,s_n(y)+\frac{L_y}{\pi n}[c_n(y)-1]\right\}e_{nC}(\tau)d\,z\,d\,y\,d\,x\,d\,\tau+\sum_{n=1}^{N}\int_0^{L_x}\left\{x\,s_n(x)+\frac{L_x}{\pi n}[c_n(x)-1]\right\}\times$$

$$\times\int_0^{L_y}\left\{y\,s_n(y)+\frac{L_y}{\pi n}[c_n(y)-1]\right\}\int_0^{L_z}\left\{z\,s_n(z)+\frac{L_z}{\pi n}[c_n(z)-1]\right\}f(x,y,z)d\,z\,d\,y\,d\,x\,.$$

As an example for $\gamma = 0$ we obtain

$$a_{nC}=\int_0^{L_x}\int_0^{L_y}\left\{y\,s_n(y)+\frac{L_y}{\pi n}[c_n(y)-1]\right\}\int_0^{L_z}\left\{z\,s_n(z)+\frac{L_y}{\pi n}[c_n(z)-1]\right\}f(x,y,z)d\,z\,d\,y\,\{x\,s_n(x)+$$

$$\times[c_n(x)-1]\frac{L_x}{\pi n}\Bigg\}d\,x\left(\frac{n}{2}\left\{\int_0^t\int_0^{L_x}s_n(2x)\int_0^{L_y}c_n(y)\left\{y\,s_n(y)+\frac{L_y}{\pi n}[c_n(y)-1]\right\}\int_0^{L_z}D_L(x,y,z,T)\times\right.\right.$$

$$\times\left\{z\,s_n(z)+\frac{L_y}{\pi n}[c_n(z)-1]\right\}\left[1+\varsigma_1\frac{V(x,y,z,\tau)}{V^*}+\varsigma_2\frac{V^2(x,y,z,\tau)}{(V^*)^2}\right]\left[1+\frac{\xi}{P^\gamma(x,y,z,T)}\right]\times$$

$$\times c_n(z)d\,z\,d\,y\,d\,x\,e_{nC}(\tau)d\,\tau+\int_0^t e_{nC}(\tau)\int_0^{L_x}c_n(x)\left\{x\,s_n(x)+\frac{L_y}{\pi n}[c_n(x)-1]\right\}\int_0^{L_y}s_n(2y)\int_0^{L_z}c_n(z)\times$$

$$\times\left\{z\,s_n(z)+\frac{L_y}{\pi n}[c_n(z)-1]\right\}\left[1+\frac{\xi}{P^\gamma(x,y,z,T)}\right]\left[1+\varsigma_1\frac{V(x,y,z,\tau)}{V^*}+\varsigma_2\frac{V^2(x,y,z,\tau)}{(V^*)^2}\right]\times$$

$$\times D_L(x,y,z,T)\,d\,z\,d\,y\,d\,x\,d\,\tau+\int_0^t e_{nC}(\tau)\int_0^{L_x}c_n(x)\left\{x\,s_n(x)+\frac{L_x}{\pi n}[c_n(x)-1]\right\}\int_0^{L_y}c_n(y)\,\{s_n(y)\times$$

$$\times y+\frac{L_y}{\pi n}[c_n(y)-1]\right\}\int_0^{L_z}s_n(2z)\,D_L(x,y,z,T)\left[1+\frac{\xi}{P^\gamma(x,y,z,T)}\right]\left[1+\varsigma_2\frac{V^2(x,y,z,\tau)}{(V^*)^2}+\right.$$

$$\left.\left.+\varsigma_1\frac{V(x,y,z,\tau)}{V^*}\right]d\,z\,d\,y\,d\,x\,d\,\tau\right\}-\frac{L_z^2L_z^2L_z^2}{\pi^5n^6}e_{nC}(t)\Bigg)^{-1}.$$

For $\gamma = 1$ one can obtain the following relation to determine required parameters

$$a_{nC}=-\frac{\beta_n}{2\alpha_n}\pm\sqrt{\beta_n^2+4\alpha_n\int_0^{L_x}c_n(x)\int_0^{L_y}c_n(y)\int_0^{L_z}c_n(z)\,f(x,y,z)d\,z\,d\,y\,d\,x}\,,$$

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where $\alpha_n = \frac{\xi L_y L_z}{2\pi^2 n}\int\limits_0^t e_{nC}(\tau)\int\limits_0^{L_x} s_n(2x)\int\limits_0^{L_y} c_n(y)\int\limits_0^{L_z}\left[1+\varsigma_1\frac{V(x,y,z,\tau)}{V^*}+\varsigma_2\frac{V^2(x,y,z,\tau)}{(V^*)^2}\right]\times$

$$\times c_n(z)\frac{D_L(x,y,z,T)}{P(x,y,z,T)}\left\{y\,s_n(y)+\frac{L_y}{\pi n}[c_n(y)-1]\right\}\left\{z\,s_n(z)+\frac{L_z}{\pi n}[c_n(z)-1]\right\}d\,z\,d\,y\,d\,x\,d\,\tau+$$

$$+\frac{\xi L_x L_z}{2\pi^2 n}\int\limits_0^t e_{nC}(\tau)\int\limits_0^{L_x} c_n(x)\left\{x\,s_n(x)+\frac{L_x}{\pi n}[c_n(x)-1]\right\}\int\limits_0^{L_y} s_n(2y)\int\limits_0^{L_z}\left\{z\,s_n(z)-\frac{L_z}{\pi n}[c_n(z)-1]\right\}\times$$

$$\times c_n(z)\frac{D_L(x,y,z,T)}{P(x,y,z,T)}\left[1+\varsigma_1\frac{V(x,y,z,\tau)}{V^*}+\varsigma_2\frac{V^2(x,y,z,\tau)}{(V^*)^2}\right]d\,z\,d\,y\,d\,x\,d\,\tau+\frac{\xi L_x L_y}{2\pi^2 n}\times$$

$$\times\int\limits_0^t e_{nC}(\tau)\int\limits_0^{L_x} c_n(x)\int\limits_0^{L_y} c_n(y)\int\limits_0^{L_z} s_n(2z)\frac{D_L(x,y,z,T)}{P(x,y,z,T)}\left[1+\varsigma_1\frac{V(x,y,z,\tau)}{V^*}+\varsigma_2\frac{V^2(x,y,z,\tau)}{(V^*)^2}\right]\times$$

$$\times\left\{x\,s_n(x)+\frac{L_x}{\pi n}[c_n(x)-1]\right\}\left\{y\,s_n(y)+\frac{L_y}{\pi n}[c_n(y)-1]\right\}d\,z\,d\,y\,d\,x\,d\,\tau,\ \beta_n=\frac{L_y L_z}{2n\pi^2}\times$$

$$\times\int\limits_0^t e_{nC}(\tau)\int\limits_0^{L_x} s_n(2x)\int\limits_0^{L_y} c_n(y)\int\limits_0^{L_z} c_n(z)D_L(x,y,z,T)\left[1+\varsigma_1\frac{V(x,y,z,\tau)}{V^*}+\varsigma_2\frac{V^2(x,y,z,\tau)}{(V^*)^2}\right]\times$$

$$\times\left\{z\,s_n(z)+\frac{L_z}{\pi n}[c_n(z)-1]\right\}d\,z\left\{y\,s_n(y)+\frac{L_y}{\pi n}[c_n(y)-1]\right\}d\,y\,d\,x\,d\,\tau+\frac{L_x L_z}{2n\pi^2}\int\limits_0^t e_{nC}(\tau)\times$$

$$\times\int\limits_0^{L_x} c_n(x)\left\{x\,s_n(x)+\frac{L_x}{\pi n}[c_n(x)-1]\right\}\int\limits_0^{L_y} s_n(2y)\int\limits_0^{L_z}\left[1+\varsigma_1\frac{V(x,y,z,\tau)}{V^*}+\varsigma_2\frac{V^2(x,y,z,\tau)}{(V^*)^2}\right]\times$$

$$\times c_n(z)D_L(x,y,z,T)\left\{z\,s_n(z)+\frac{L_z}{\pi n}[c_n(z)-1]\right\}d\,z\,d\,y\,d\,x\,d\,\tau+\frac{L_x L_y}{2n\pi^2}\int\limits_0^t e_{nC}(\tau)\int\limits_0^{L_x}\{x\,s_n(x)+$$

$$+\frac{L_x}{\pi n}[c_n(x)-1]\right\}\int\limits_0^{L_y}\left\{y\,s_n(y)+\frac{L_y}{\pi n}[c_n(y)-1]\right\}\int\limits_0^{L_z}\left[1+\varsigma_1\frac{V(x,y,z,\tau)}{V^*}+\varsigma_2\frac{V^2(x,y,z,\tau)}{(V^*)^2}\right]\times$$

$$\times s_n(2z)D_L(x,y,z,T)\,d\,z\,c_n(y)d\,y\,c_n(x)d\,x\,d\,\tau-L_x^2L_y^2L_z^2e_{nC}(t)/\pi^5n^6\,.$$

Analogous way could be used to calculate values of parameters a_n for larger values of parameter γ. However the relations will not be present in the paper because the relations are bulky. Advantage of the approach is absent of necessity to join dopant concentration on interfaces of heterostructure.

Equations of the system (4) have been also solved by using Bubnov-Galerkin approach. Previously we transform the differential equations to the following integro- differential form

$$\begin{cases}\frac{xyz}{L_xL_yL_z}\int\limits_{L_x}^{x}\int\limits_{L_y}^{y}\int\limits_{L_z}^{z} I(u,v,w,t)\,d\,w\,d\,v\,d\,u=\int\limits_0^t\int\limits_{L_y}^{y}\int\limits_{L_z}^{z} D_I(x,v,w,T)\frac{\partial I(x,v,w,\tau)}{\partial x}d\,w\,d\,v\,d\,\tau\times\\ \times\frac{yz}{L_yL_z}+\frac{xz}{L_xL_z}\int\limits_0^t\int\limits_{L_x}^{x}\int\limits_{L_z}^{z} D_I(u,y,w,T)\frac{\partial I(u,y,w,\tau)}{\partial x}d\,w\,d\,u\,d\,\tau-\int\limits_{L_x}^{x}\int\limits_{L_y}^{y}\int\limits_{L_z}^{z} k_{I,V}(u,v,w,T)\times\\ \times I(u,v,w,t)V(u,v,w,t)\,d\,w\,d\,v\,d\,u\frac{xyz}{L_xL_yL_z}+\frac{xy}{L_xL_y}\int\limits_0^t\int\limits_{L_x}^{x}\int\limits_{L_y}^{y}\frac{\partial I(u,v,z,\tau)}{\partial z}\times\\ \times D_I(u,v,z,T)\,d\,v\,d\,u\,d\,\tau-\frac{xyz}{L_xL_yL_z}\int\limits_{L_x}^{x}\int\limits_{L_y}^{y}\int\limits_{L_z}^{z} k_{I,I}(u,v,w,T)I^2(u,v,w,t)\,d\,w\,d\,v\,d\,u+\\ +\frac{xyz}{L_xL_yL_z}\int\limits_{L_x}^{x}\int\limits_{L_y}^{y}\int\limits_{L_z}^{z} f_I(u,v,w)\,d\,w\,d\,v\,d\,u\\ \frac{xyz}{L_xL_yL_z}\int\limits_{L_x}^{x}\int\limits_{L_y}^{y}\int\limits_{L_z}^{z} V(u,v,w,t)\,d\,w\,d\,v\,d\,u=\int\limits_0^t\int\limits_{L_y}^{y}\int\limits_{L_z}^{z} D_V(x,v,w,T)\frac{\partial V(x,v,w,\tau)}{\partial x}d\,w\,d\,v\,d\,\tau\times\\ \times\frac{yz}{L_yL_z}+\frac{xz}{L_xL_z}\int\limits_0^t\int\limits_{L_x}^{x}\int\limits_{L_z}^{z} D_V(u,y,w,T)\frac{\partial V(u,y,w,\tau)}{\partial x}d\,w\,d\,u\,d\,\tau+\int\limits_0^t\int\limits_{L_x}^{x}\int\limits_{L_y}^{y} D_V(u,v,z,T)\times\\ \times\frac{\partial V(u,v,z,\tau)}{\partial z}d\,v\,d\,u\,d\,\tau\frac{xy}{L_xL_y}-\frac{xyz}{L_xL_yL_z}\int\limits_{L_x}^{x}\int\limits_{L_y}^{y}\int\limits_{L_z}^{z} k_{I,V}(u,v,w,T)I(u,v,w,t)\times\\ \times V(u,v,w,t)\,d\,w\,d\,v\,d\,u-\frac{xyz}{L_xL_yL_z}\int\limits_{L_x}^{x}\int\limits_{L_y}^{y}\int\limits_{L_z}^{z} k_{V,V}(u,v,w,T)V^2(u,v,w,t)\,d\,w\,d\,v\,d\,u+\\ +\frac{xyz}{L_xL_yL_z}\int\limits_{L_x}^{x}\int\limits_{L_y}^{y}\int\limits_{L_z}^{z} f_V(u,v,w)\,d\,w\,d\,v\,d\,u\end{cases}\tag{4a}$$

Farther we determine solutions of the above equations as the following series

$$\rho_0(x,y,z,t)=\sum_{n=1}^{N}a_{n\rho}\,c_n(x)\,c_n(y)\,c_n(z)\,e_{n\rho}(t),$$

where $a_{n\rho}$ are not yet known coefficients. Substitution of the series into Eqs.(4a) leads to the following results

$$\frac{xyz}{\pi^3}\sum_{n=1}^{N}\frac{a_{nI}}{n^3}s_n(x)\,s_n(y)\,s_n(z)\,e_{nI}(t)=-\frac{yz\pi}{L_xL_yL_z}\sum_{n=1}^{N}a_{nI}\int\limits_0^t\int\limits_{L_y}^{y}c_n(y)\int\limits_{L_z}^{z}c_n(z)D_I(x,v,w,T)\,d\,w\,d\,v\times$$

$$\times e_{nI}(\tau)\,d\,\tau\;s_n(x)-\frac{xz\pi}{L_xL_yL_z}\sum_{n=1}^{N}a_{nI}\,s_n(y)\int\limits_0^t e_{nI}(\tau)\int\limits_{L_x}^{x}c_n(x)\int\limits_{L_z}^{z}c_n(z)D_I(u,y,w,T)\,d\,w\,d\,u\,d\,\tau-$$

$$-\frac{x\,y\,\pi}{L_xL_yL_z}\sum_{n=1}^{N}a_{nI}s_n(z)\int_0^t e_{nI}(\tau)\int_{L_x}^{x}c_n(x)\int_{L_y}^{y}c_n(y)D_I(u,v,z,T)\,d\,v\,d\,u\,d\,\tau-\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}k_{I,I}(u,v,v,T)\times$$

$$\times\left[\sum_{n=1}^{N}a_{nI}\,c_n(u)\,c_n(v)\,c_n(w)\,e_{nI}(t)\right]^2 d\,w\,d\,v\,d\,u\frac{x\,y\,z}{L_xL_yL_z}-\frac{x\,y\,z}{L_xL_yL_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}\sum_{n=1}^{N}a_{nI}\,c_n(u)\,c_n(v)\,c_n(w)\times$$

$$\times\,e_{nI}(t)\sum_{n=1}^{N}a_{nV}\,c_n(u)\,c_n(v)\,c_n(w)\,e_{nV}(t)k_{I,V}(u,v,v,T)\,d\,w\,d\,v\,d\,u+\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}f_I(u,v,w)\,d\,w\,d\,v\,d\,u\times$$

$$\times\,x\,y\,z/L_xL_yL_z$$

$$\frac{x\,y\,z}{\pi^3}\sum_{n=1}^{N}\frac{a_{nV}}{n^3}s_n(x)\,s_n(y)\,s_n(z)\,e_{nV}(t)=-\frac{y\,z\,\pi}{L_xL_yL_z}\sum_{n=1}^{N}a_{nV}\int_0^t\int_{L_y}^{y}c_n(y)\int_{L_z}^{z}c_n(z)D_V(x,v,w,T)\,d\,w\,d\,v\times$$

$$\times\,e_{nV}(\tau)\,d\,\tau\;s_n(x)-\frac{x\,z\,\pi}{L_xL_yL_z}\sum_{n=1}^{N}a_{nV}\,s_n(y)\int_0^t e_{nV}(\tau)\int_{L_x}^{x}c_n(x)\int_{L_z}^{z}c_n(z)D_V(u,y,w,T)\,d\,w\,d\,u\,d\,\tau-$$

$$-\frac{x\,y\,\pi}{L_xL_yL_z}\sum_{n=1}^{N}a_{nV}s_n(z)\int_0^t e_{nV}(\tau)\int_{L_x}^{x}c_n(x)\int_{L_y}^{y}c_n(y)D_V(u,v,z,T)\,d\,v\,d\,u\,d\,\tau-\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}k_{V,V}(u,v,v,T)\times$$

$$\times\left[\sum_{n=1}^{N}a_{nV}\,c_n(u)\,c_n(v)\,c_n(w)\,e_{nI}(t)\right]^2 d\,w\,d\,v\,d\,u\frac{x\,y\,z}{L_xL_yL_z}-\frac{x\,y\,z}{L_xL_yL_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}\sum_{n=1}^{N}a_{nI}c_n(u)\,c_n(v)\,c_n(w)\times$$

$$\times\,e_{nI}(t)\sum_{n=1}^{N}a_{nV}\,c_n(u)\,c_n(v)\,c_n(w)\,e_{nV}(t)k_{I,V}(u,v,v,T)\,d\,w\,d\,v\,d\,u+\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}f_V(u,v,w)\,d\,w\,d\,v\,d\,u\times$$

$$\times\,x\,y\,z/L_xL_yL_z\,.$$

We determine coefficients $a_{n\rho}$ by using orthogonality condition on the scale of heterostructure. The condition gives us possibility to obtain relations to calculate $a_{n\rho}$ for any quantity N of terms of considered series. In the common case equations for the required coefficients could be written as

$$-\frac{L_x^2L_y^2L_z^2}{\pi^5}\sum_{n=1}^{N}\frac{a_{nI}}{n^6}e_{nI}(t)=-\frac{1}{2\pi\,L_x}\sum_{n=1}^{N}\frac{a_{nI}}{n^2}\int_0^t\int_0^{L_x}[1-c_n(2x)]\int_0^{L_y}\left\{L_y+y\,s_n(2y)+\frac{L_y}{2\pi\,n}[c_n(2y)-1]\right\}\times$$

$$\times\int_0^{L_z}D_I(x,y,z,T)\left\{z\,s_n(z)+\frac{L_z}{2\pi\,n}[c_n(z)-1]\right\}d\,z\,d\,y\,d\,x\,e_{nI}(\tau)\,d\,\tau-\frac{1}{2\pi\,L_y}\sum_{n=1}^{N}\frac{a_{nI}}{n^2}\int_0^t\int_0^{L_x}\{\,x\,s_n(2x)+$$

$$+L_x+\frac{L_x}{\pi\,n}[c_n(2x)-1]\right\}\int_0^{L_y}\int_0^{L_z}D_I(x,y,z,T)\left\{L_z+z\,s_n(2z)+\frac{L_z}{2\pi\,n}[c_n(2z)-1]\right\}d\,z[1-c_n(2y)]\times$$

$$\times\,d\,y\,d\,x\,e_{nI}(\tau)\,d\,\tau\int_0^{L_z}D_I(x,y,z,T)\left\{L_z+z\,s_n(2z)+\frac{L_z}{2\pi\,n}[c_n(2z)-1]\right\}d\,z\,d\,y\,d\,x\,e_{nI}(\tau)\,d\,\tau-$$

$$-\frac{1}{2\pi L_z}\sum_{n=1}^{N}\frac{a_{nI}}{n^2}\int_0^t\int_0^{L_x}\left\{L_x+x\,s_n(2x)+\frac{L_x}{2\pi n}\left[c_n(2x)-1\right]\right\}\int_0^{L_y}\left\{L_y+y\,s_n(2y)+\frac{L_y}{2\pi n}\left[c_n(2y)-1\right]\right\}\times$$

$$\times\int_0^{L_z}\left[1-c_n(2z)\right]D_I(x,y,z,T)\,d\,z\,d\,y\,d\,x\,e_{nI}(\tau)\,d\,\tau-\sum_{n=1}^{N}a_{nI}^2e_{nI}(2t)\int_0^{L_x}\left\{L_x+\frac{L_x}{2\pi n}\left[c_n(2x)-1\right]+\right.$$

$$\left.+x\,s_n(2x)\right\}\int_0^{L_y}\left\{L_y+y\,s_n(2y)+\frac{L_y}{2\pi n}\left[c_n(2y)-1\right]\right\}\int_0^{L_z}k_{I,I}(x,y,z,T)\left\{L_z+\frac{L_z}{2\pi n}\left[c_n(2z)-1\right]+\right.$$

$$\left.+z\,s_n(2z)\right\}d\,z\,d\,y\,d\,x-\sum_{n=1}^{N}a_{nI}a_{nV}e_{nI}(t)e_{nV}(t)\int_0^{L_x}\left\{L_x+x\,s_n(2x)+\frac{L_x}{2\pi n}\left[c_n(2x)-1\right]\right\}\int_0^{L_y}\left\{L_y+\right.$$

$$\left.+y\,s_n(2y)+\frac{L_y}{2\pi n}\left[c_n(2y)-1\right]\right\}\int_0^{L_z}k_{I,V}(x,y,z,T)\left\{L_z+z\,s_n(2z)+\frac{L_z}{2\pi n}\left[c_n(2z)-1\right]\right\}d\,z\,\times$$

$$\times\,d\,y\,d\,x+\sum_{n=1}^{N}\int_0^{L_x}\left\{x\,s_n(x)+\frac{L_x}{\pi n}\left[c_n(x)-1\right]\right\}\int_0^{L_y}\left\{y\,s_n(y)+\frac{L_y}{\pi n}\left[c_n(y)-1\right]\right\}\int_0^{L_z}f_I(x,y,z,T)\times$$

$$\times\left\{L_z+z\,s_n(2z)+\frac{L_z}{2\pi n}\left[c_n(2z)-1\right]\right\}d\,z\,d\,y\,d\,x$$

$$-\frac{L_x^2L_y^2L_z^2}{\pi^5}\sum_{n=1}^{N}\frac{a_{nV}}{n^6}e_{nV}(t)=-\frac{1}{2\pi L_x}\sum_{n=1}^{N}\frac{a_{nV}}{n^2}\int_0^t\int_0^{L_x}\left[1-c_n(2x)\right]\int_0^{L_y}\left\{L_y+y\,s_n(2y)+\frac{L_y}{2\pi n}\left[c_n(2y)-1\right]\right\}\times$$

$$\times\int_0^{L_z}D_V(x,y,z,T)\left\{z\,s_n(z)+\frac{L_z}{2\pi n}\left[c_n(z)-1\right]\right\}d\,z\,d\,y\,d\,x\,e_{nV}(\tau)\,d\,\tau-\frac{1}{2\pi L_y}\sum_{n=1}^{N}\frac{a_{nV}}{n^2}\int_0^t\int_0^{L_x}\left\{x\,s_n(2x)+\right.$$

$$\left.+L_x+\frac{L_x}{\pi n}\left[c_n(2x)-1\right]\right\}\int_0^{L_y}\int_0^{L_z}D_V(x,y,z,T)\left\{L_z+z\,s_n(2z)+\frac{L_z}{2\pi n}\left[c_n(2z)-1\right]\right\}d\,z\left[1-c_n(2y)\right]\times$$

$$\times\,d\,y\,d\,x\,e_{nV}(\tau)\,d\,\tau\int_0^{L_z}D_V(x,y,z,T)\left\{L_z+z\,s_n(2z)+\frac{L_z}{2\pi n}\left[c_n(2z)-1\right]\right\}d\,z\,d\,y\,d\,x\,e_{nV}(\tau)\,d\,\tau-$$

$$-\frac{1}{2\pi L_z}\sum_{n=1}^{N}\frac{a_{nV}}{n^2}\int_0^t\int_0^{L_x}\left\{L_x+x\,s_n(2x)+\frac{L_x}{2\pi n}\left[c_n(2x)-1\right]\right\}\int_0^{L_y}\left\{L_y+y\,s_n(2y)+\frac{L_y}{2\pi n}\left[c_n(2y)-1\right]\right\}\times$$

$$\times\int_0^{L_z}\left[1-c_n(2z)\right]D_V(x,y,z,T)\,d\,z\,d\,y\,d\,x\,e_{nV}(\tau)\,d\,\tau-\sum_{n=1}^{N}a_{nV}^2e_{nV}(2t)\int_0^{L_x}\left\{L_x+\frac{L_x}{2\pi n}\left[c_n(2x)-1\right]+\right.$$

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$$+x\,s_n(2x)\Big\}\int_0^{L_y}\left\{L_y+y\,s_n(2y)+\frac{L_y}{2\pi n}[c_n(2y)-1]\right\}\int_0^{L_z}k_{V,V}(x,y,z,T)\left\{L_z+\frac{L_z}{2\pi n}[c_n(2z)-1]+\right.$$

$$\left.+z\,s_n(2z)\right\}d\,z\,d\,y\,d\,x-\sum_{n=1}^{N}a_{nI}a_{nV}e_{nI}(t)e_{nV}(t)\int_0^{L_x}\left\{L_x+x\,s_n(2x)+\frac{L_x}{2\pi n}[c_n(2x)-1]\right\}\int_0^{L_y}\Big\{L_y+$$

$$+y\,s_n(2y)+\frac{L_y}{2\pi n}[c_n(2y)-1]\Big\}\int_0^{L_z}k_{I,V}(x,y,z,T)\left\{L_z+z\,s_n(2z)+\frac{L_z}{2\pi n}[c_n(2z)-1]\right\}d\,z\times$$

$$\times d\,y\,d\,x+\sum_{n=1}^{N}\int_0^{L_x}\left\{x\,s_n(x)+\frac{L_x}{\pi n}[c_n(x)-1]\right\}\int_0^{L_y}\left\{y\,s_n(y)+\frac{L_y}{\pi n}[c_n(y)-1]\right\}\int_0^{L_z}f_V(x,y,z,T)\times$$

$$\times\left\{L_z+z\,s_n(2z)+\frac{L_z}{2\pi n}[c_n(2z)-1]\right\}d\,z\,d\,y\,d\,x\,.$$

In the final form relations for required parameters could be written as

$$a_{nI}=-\frac{b_3+A}{4b_4}\pm\sqrt{\frac{(b_3+A)^2}{4}-4b_4\left(y+\frac{b_3y-\gamma_{nV}\lambda_{nI}^2}{A}\right)},\quad a_{nV}=-\frac{\gamma_{nI}a_{nI}^2+\delta_{nI}a_{nI}+\lambda_{nI}}{\chi_{nI}a_{nI}},$$

where $\gamma_{n\rho}=e_{n\rho}(2t)\int_0^{L_x}\int_0^{L_y}\int_0^{L_z}k_{\rho,\rho}(x,y,z,T)\left\{L_x+x\,s_n(2x)+\frac{L_x}{2\pi n}[c_n(2x)-1]\right\}\Big\{y\,s_n(2y)+L_y+$

$$+\frac{L_y}{2\pi n}[c_n(2y)-1]\Big\}\left\{L_z+z\,s_n(2z)+\frac{L_z}{2\pi n}[c_n(2z)-1]\right\}d\,z\,d\,y\,d\,x\,,\quad \delta_{n\rho}=\frac{1}{2\pi L_x n^2}\int_0^t e_{n\rho}(\tau)\times$$

$$\times\int_0^{L_x}\int_0^{L_y}\left\{y\,s_n(y)+\frac{L_y}{2\pi n}[c_n(y)-1]\right\}\int_0^{L_z}\left\{z\,s_n(z)+\frac{L_z}{2\pi n}[c_n(z)-1]\right\}D_\rho(x,y,z,T)\,d\,z\,d\,y\,[1-$$

$$-c_n(2x)]\,d\,x\,d\,\tau+\frac{1}{2\pi L_y n^2}\int_0^t e_{n\rho}(\tau)\int_0^{L_x}\left\{L_x+x\,s_n(2x)+\frac{L_x}{\pi n}[c_n(2x)-1]\right\}\int_0^{L_y}[1-c_n(2y)]\int_0^{L_z}\Big\{L_z+$$

$$+z\,s_n(2z)+\frac{L_z}{2\pi n}[c_n(2z)-1]\Big\}D_\rho(x,y,z,T)\,d\,z\,d\,y\,d\,x\,d\,\tau+\frac{1}{2\pi L_z n^2}\int_0^t e_{n\rho}(\tau)\int_0^{L_x}\Big\{x\,s_n(2x)+$$

$$+L_x+\frac{L_x}{\pi n}[c_n(2x)-1]\Big\}\int_0^{L_y}\left\{L_y+y\,s_n(y)+\frac{L_y}{2\pi n}[c_n(y)-1]\right\}\int_0^{L_z}[1-c_n(2z)]D_\rho(x,y,z,T)\,d\,z\times$$

$$\times d\,y\,d\,x\,d\,\tau-\frac{L_x^2L_y^2L_z^2}{\pi^5n^6}e_{n\rho}(t),\ \chi_{nIV}=\int_0^{L_x}\left\{x\,s_n(x)+\frac{L_x}{\pi n}[c_n(x)-1]\right\}\int_0^{L_y}\left\{L_y+\frac{L_y}{2\pi n}[c_n(2y)-1]+\right.$$

$$+ y s_n(2y)\}\int_0^{L_z} k_{I,V}(x,y,z,T)\left\{L_z + z s_n(2z) + \frac{L_z}{2\pi n}[c_n(2z)-1]\right\} d z\, d y\, d x\, e_{nI}(t)\, e_{nV}(t),$$

$$\lambda_{n\rho} = \int_0^{L_x}\left\{x s_n(x) + \frac{L_x}{\pi n}[c_n(x)-1]\right\}\int_0^{L_y}\left\{y s_n(y) + \frac{L_y}{\pi n}[c_n(y)-1]\right\}\int_0^{L_z}\left\{z s_n(z) + \frac{L_z}{\pi n}[c_n(z)-1]\right\} \times$$

$$\times f_\rho(x,y,z,T)\, d z\, d y\, d x,\ b_4 = \gamma_{nV}\gamma_{nI}^2 - \gamma_{nI}\chi_{nI}^2,\ b_3 = 2\gamma_{nV}\gamma_{nI}\delta_{nI} - \delta_{nI}\chi_{nI}^2 - \delta_{nV}\chi_{nI}\gamma_{nI},$$

$$A = \sqrt{8y + b_3^2 - 4b_2},\ b_2 = \gamma_{nV}\delta_{nI}^2 + 2\lambda_{nI}\gamma_{nV}\gamma_{nI} - \delta_{nV}\chi_{nI}\delta_{nI} + (\lambda_{nV} - \lambda_{nI})\chi_{nI}^2,\ b_1 = 2\lambda_{nI} \times$$

$$\times \gamma_{nV}\delta_{nI} - \delta_{nV}\chi_{nI}\lambda_{nI},\ y = \sqrt[3]{\sqrt{q^2 + p^3} - q} - \sqrt[3]{\sqrt{q^2 + p^3} + q} - \frac{b_3}{3b_4},\ p = \frac{3b_2 b_4 - b_3^2}{9b_4^2},$$

$$q = \left(2b_3^3 - 9b_2 b_3 + 27b_1 b_4^2\right)/54 b_4^3.$$

We determine spatio-temporal distributions of concentrations of complexes of radiation defects in the following form

$$\Phi_{\rho 0}(x,y,z,t) = \sum_{n=1}^{N} a_{n\Phi\rho}\, c_n(x)\, c_n(y)\, c_n(z)\, e_{n\rho}(t),$$

where $a_{n\Phi\rho}$ are not yet known coefficients. Let us previously transform the Eqs.(6) to the following integro-differential form

$$\frac{xyz}{L_x L_y L_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}\Phi_I(u,v,w,t)\, d w\, d v\, d u = \int_0^t\int_{L_y}^{y}\int_{L_z}^{z} D_{\Phi I}(x,v,w,T)\frac{\partial \Phi_I(x,v,w,\tau)}{\partial x} d w\, d v\, d\tau \times$$

$$\times \frac{yz}{L_y L_z} + \frac{xz}{L_x L_z}\int_0^t\int_{L_x}^{x}\int_{L_z}^{z} D_{\Phi I}(u,y,w,T)\frac{\partial \Phi_I(u,y,w,\tau)}{\partial y} d w\, d u\, d\tau + \frac{xy}{L_x L_y}\int_0^t\int_{L_x}^{x}\int_{L_y}^{y} D_{\Phi I}(u,v,z,T) \times$$

$$\times \frac{\partial \Phi_I(u,v,z,\tau)}{\partial z} d v\, d u\, d\tau + \frac{xyz}{L_x L_y L_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z} k_{I,I}(u,v,w,T) I^2(u,v,w,\tau)\, d w\, d v\, d u - \quad \textbf{(6a)}$$

$$- \frac{xyz}{L_x L_y L_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z} k_I(u,v,w,T)\, I(u,v,w,\tau)\, d w\, d v\, d u + \frac{xyz}{L_x L_y L_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z} f_{\Phi I}(u,v,w)\, d w\, d v\, d u$$

$$\frac{xyz}{L_x L_y L_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}\Phi_V(u,v,w,t)\, d w\, d v\, d u = \int_0^t\int_{L_y}^{y}\int_{L_z}^{z} D_{\Phi V}(x,v,w,T)\frac{\partial \Phi_V(x,v,w,\tau)}{\partial x} d w\, d v\, d\tau \times$$

$$\times \frac{yz}{L_y L_z} + \frac{xz}{L_x L_z}\int_0^t\int_{L_x}^{x}\int_{L_z}^{z} D_{\Phi V}(u,y,w,T)\frac{\partial \Phi_V(u,y,w,\tau)}{\partial y} d w\, d u\, d\tau + \frac{xy}{L_x L_y}\int_0^t\int_{L_x}^{x}\int_{L_y}^{y} D_{\Phi V}(u,v,z,T) \times$$

$$\times \frac{\partial \Phi_V(u,v,z,\tau)}{\partial z} d v\, d u\, d\tau + \frac{xyz}{L_x L_y L_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z} k_{V,V}(u,v,w,T) V^2(u,v,w,\tau)\, d w\, d v\, d u -$$

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$$-\frac{x\,y\,z}{L_x L_y L_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}k_V(u,v,w,T)\,V(u,v,w,\tau)\,d\,w\,d\,v\,d\,u+\frac{x\,y\,z}{L_x L_y L_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}f_{\Phi V}(u,v,w)\,d\,w\,d\,v\,d\,u\,.$$

Substitution of the previously considered series in the Eqs.(6a) leads to the following form

$$-x\,y\,z\sum_{n=1}^{N}\frac{a_{n\Phi I}}{\pi^3 n^3}s_n(x)\,s_n(y)\,s_n(z)\,e_{nI}(t)=-\frac{y\,z\,\pi}{L_x L_y L_z}\sum_{n=1}^{N}n\,a_{n\Phi I}\,s_n(x)e_{nI}(t)\int_0^t\int_{L_y}^{y}\int_{L_z}^{z}c_n(v)c_n(w)\times$$

$$\times D_{\Phi I}(x,v,w,T)\,d\,w\,d\,v\,d\,\tau-\frac{x\,z\,\pi}{L_x L_y L_z}\sum_{n=1}^{N}a_{n\Phi I}\int_0^t\int_{L_x}^{x}\int_{L_z}^{z}c_n(u)c_n(w)\,D_{\Phi I}(u,v,w,T)\,d\,w\,d\,u\,d\,\tau\times$$

$$\times n\,s_n(y)e_{n\Phi I}(t)-\frac{x\,y\,\pi}{L_x L_y L_z}\sum_{n=1}^{N}n\,a_{n\Phi I}\,s_n(z)e_{n\Phi I}(t)\int_0^t\int_{L_x}^{x}\int_{L_y}^{y}c_n(u)c_n(v)\,D_{\Phi I}(u,v,z,T)\,d\,v\,d\,u\,d\,\tau+$$

$$+\frac{x\,y\,z}{L_x L_y L_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}k_{I,I}(u,v,w,T)\,I^2(u,v,w,\tau)\,d\,w\,d\,v\,d\,u+\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}f_{\Phi I}(u,v,w)\,d\,w\,d\,v\,d\,u\times$$

$$\times\frac{x\,y\,z}{L_x L_y L_z}-\frac{x\,y\,z}{L_x L_y L_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}k_I(u,v,w,T)\,I(u,v,w,\tau)\,d\,w\,d\,v\,d\,u$$

$$-x\,y\,z\sum_{n=1}^{N}\frac{a_{n\Phi V}}{\pi^3 n^3}s_n(x)\,s_n(y)\,s_n(z)\,e_{nV}(t)=-\frac{y\,z\,\pi}{L_x L_y L_z}\sum_{n=1}^{N}n\,a_{n\Phi V}\,s_n(x)e_{nV}(t)\int_0^t\int_{L_y}^{y}\int_{L_z}^{z}c_n(v)c_n(w)\times$$

$$\times D_{\Phi V}(x,v,w,T)\,d\,w\,d\,v\,d\,\tau-\frac{x\,z\,\pi}{L_x L_y L_z}\sum_{n=1}^{N}n\int_0^t\int_{L_x}^{x}\int_{L_z}^{z}c_n(u)c_n(w)\,D_{\Phi V}(u,v,w,T)\,d\,w\,d\,u\,d\,\tau\times$$

$$\times a_{n\Phi V}\,s_n(y)e_{n\Phi V}(t)-\frac{x\,y\,\pi}{L_x L_y L_z}\sum_{n=1}^{N}n\,s_n(z)e_{n\Phi V}(t)\int_0^t\int_{L_x}^{x}\int_{L_y}^{y}c_n(u)c_n(v)\,D_{\Phi V}(u,v,z,T)\,d\,v\,d\,u\,d\,\tau\times$$

$$\times a_{n\Phi V}+\frac{x\,y\,z}{L_x L_y L_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}k_{V,V}(u,v,w,T)\,V^2(u,v,w,\tau)\,d\,w\,d\,v\,d\,u+\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}f_{\Phi V}(u,v,w)\,d\,w\,d\,v\,d\,u\times$$

$$\times\frac{x\,y\,z}{L_x L_y L_z}-\frac{x\,y\,z}{L_x L_y L_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}k_V(u,v,w,T)\,V(u,v,w,\tau)\,d\,w\,d\,v\,d\,u\,.$$

We determine coefficients $a_{n\Phi\rho}$ by using orthogonality condition on the scale of heterostructure. The condition gives us possibility to obtain relations to calculate $a_{n\Phi\rho}$ for any quantity N of terms of considered series. In the common case equations for the required coefficients could be written as

$$-\frac{L_x^2L_y^2L_z^2}{\pi^5}\sum_{n=1}^{N}\frac{a_{n\Phi I}}{n^6}e_{n\Phi I}(t)=-\frac{1}{2\pi\,L_x}\sum_{n=1}^{N}\int_0^t\int_0^{L_x}[1-c_n(2x)]\int_0^{L_y}\left\{L_y+y\,s_n(2y)+\frac{L_y}{2\pi\,n}[c_n(2y)-1]\right\}\times$$

$$\times\frac{a_{n\Phi I}}{n^2}\int_0^{L_z}D_{\Phi I}(x,y,z,T)\left\{z\,s_n(z)+\frac{L_z}{2\pi\,n}[c_n(z)-1]\right\}d\,z\,d\,y\,d\,x\,e_{n\Phi I}(\tau)\,d\,\tau-\frac{1}{2\pi}\sum_{n=1}^{N}\int_0^t\int_0^{L_x}\{x\,s_n(2x)+$$

$$+L_x+\frac{L_x}{2\pi n}\left[c_n(2x)-1\right]\Bigg\}\int_0^{L_y}\left[1-c_n(2y)\right]\int_0^{L_z}D_{\Phi I}(x,y,z,T)\left\{z\,s_n(z)+\frac{L_z}{2\pi n}\left[c_n(z)-1\right]\right\}d\,z\,d\,y\,d\,x\times$$

$$\times\,a_{n\Phi I}\,\frac{e_{n\Phi I}(\tau)}{n^2L_y}d\,\tau-\frac{1}{2\pi L_x}\sum_{n=1}^{N}\frac{a_{n\Phi I}}{n^2}\int_0^t\int_0^{L_x}\left\{x\,s_n(x)+\frac{L_x}{2\pi n}\left[c_n(x)-1\right]\right\}\int_0^{L_y}\left\{y\,s_n(2y)+\frac{L_y}{2\pi n}\left[c_n(2y)-1\right]+\right.$$

$$\left.+L_y\right\}\int_0^{L_z}\left[1-c_n(2y)\right]D_{\Phi I}(x,y,z,T)\,d\,z\,d\,y\,d\,x\;e_{n\Phi I}(\tau)\,d\,\tau+\frac{1}{\pi^3}\sum_{n=1}^{N}\frac{a_{n\Phi I}}{n^3}\int_0^t e_{n\Phi I}(\tau)\int_0^{L_x}\left\{\frac{L_x}{2\pi n}\left[c_n(x)-1\right]+\right.$$

$$\left.+x\,s_n(x)\right\}\int_0^{L_y}\left\{y\,s_n(y)+\frac{L_y}{2\pi n}\left[c_n(y)-1\right]\right\}\int_0^{L_z}I^2(x,y,z,t)\,k_{I,I}(x,y,z,T)\left\{\frac{L_z}{2\pi n}\left[c_n(z)-1\right]+\right.$$

$$\left.+z\,s_n(z)\right\}d\,z\,d\,y\,d\,x-\frac{1}{\pi^3}\sum_{n=1}^{N}\frac{a_{n\Phi I}}{n^3}\int_0^t e_{n\Phi I}(\tau)\int_0^{L_x}\left\{x\,s_n(x)+\frac{L_x}{2\pi n}\left[c_n(x)-1\right]\right\}\int_0^{L_y}\left\{\frac{L_y}{2\pi n}\left[c_n(y)-1\right]+\right.$$

$$\left.+y\,s_n(y)\right\}\int_0^{L_z}\left\{z\,s_n(z)+\frac{L_z}{2\pi n}\left[c_n(z)-1\right]\right\}k_I(x,y,z,T)\,I\,(x,y,z,t)\,d\,z\,d\,y\,d\,x+\frac{1}{\pi^3}\sum_{n=1}^{N}\frac{a_{n\Phi I}}{n^3}\times$$

$$\times\int_0^t e_{n\Phi I}(\tau)\int_0^{L_x}\left\{x\,s_n(x)+\frac{L_x}{2\pi n}\left[c_n(x)-1\right]\right\}\int_0^{L_y}\left\{y\,s_n(y)+\frac{L_y}{2\pi n}\left[c_n(y)-1\right]\right\}\int_0^{L_z}\left\{\frac{L_z}{2\pi n}\left[c_n(z)-1\right]+\right.$$

$$\left.+z\,s_n(z)\right\}f_{\Phi I}(x,y,z)\,d\,z\,d\,y\,d\,x$$

$$-\frac{L_x^2L_y^2L_z^2}{\pi^5}\sum_{n=1}^{N}\frac{a_{n\Phi V}}{n^6}e_{n\Phi V}(t)=-\frac{1}{2\pi L_x}\sum_{n=1}^{N}\int_0^t\int_0^{L_x}\left[1-c_n(2x)\right]\int_0^{L_y}\left\{L_y+y\,s_n(2y)+\frac{L_y}{2\pi n}\left[c_n(2y)-1\right]\right\}\times$$

$$\times\frac{a_{n\Phi V}}{n^2}\int_0^{L_z}D_{\Phi V}(x,y,z,T)\left\{z\,s_n(z)+\frac{L_z}{2\pi n}\left[c_n(z)-1\right]\right\}d\,z\,d\,y\,d\,x\,e_{n\Phi V}(\tau)\;d\,\tau-\frac{1}{2\pi}\sum_{n=1}^{N}\int_0^t\int_0^{L_x}\left\{x\,s_n(2x)+\right.$$

$$+L_x+\frac{L_x}{2\pi n}\left[c_n(2x)-1\right]\Bigg\}\int_0^{L_y}\left[1-c_n(2y)\right]\int_0^{L_z}D_{\Phi V}(x,y,z,T)\left\{z\,s_n(z)+\frac{L_z}{2\pi n}\left[c_n(z)-1\right]\right\}d\,z\,d\,y\,d\,x\times$$

$$\times\,a_{n\Phi V}\,\frac{e_{n\Phi V}(\tau)}{n^2L_y}d\,\tau-\frac{1}{2\pi L_x}\sum_{n=1}^{N}\frac{a_{n\Phi V}}{n^2}\int_0^t\int_0^{L_x}\left\{x\,s_n(x)+\frac{L_x}{2\pi n}\left[c_n(x)-1\right]\right\}\int_0^{L_y}\left\{y\,s_n(2y)+\frac{L_y}{2\pi n}\left[c_n(2y)-1\right]+\right.$$

$$\left.+L_y\right\}\int_0^{L_z}\left[1-c_n(2y)\right]D_{\Phi V}(x,y,z,T)\,d\,z\,d\,y\,d\,x\;e_{n\Phi V}(\tau)\,d\,\tau+\frac{1}{\pi^3}\sum_{n=1}^{N}\frac{a_{n\Phi V}}{n^3}\int_0^t e_{n\Phi V}(\tau)\int_0^{L_x}\left\{\frac{L_x}{2\pi n}\left[c_n(x)-1\right]+\right.$$

$$\left.+x\,s_n(x)\right\}\int_0^{L_y}\left\{y\,s_n(y)+\frac{L_y}{2\pi n}\left[c_n(y)-1\right]\right\}\int_0^{L_z}V^2(x,y,z,t)\,k_{V,V}(x,y,z,T)\left\{\frac{L_z}{2\pi n}\left[c_n(z)-1\right]+\right.$$

$$+z\,s_n(z)\}\,d\,z\,d\,y\,d\,x-\frac{1}{\pi^3}\sum_{n=1}^{N}\frac{a_{n\Phi V}}{n^3}\int_0^t e_{n\Phi V}(\tau)\int_0^{L_x}\left\{x\,s_n(x)+\frac{L_x}{2\pi n}[c_n(x)-1]\right\}\int_0^{L_y}\left\{\frac{L_y}{2\pi n}[c_n(y)-1]+\right.$$

$$\left.+y\,s_n(y)\right\}\int_0^{L_z}\left\{z\,s_n(z)+\frac{L_z}{2\pi n}[c_n(z)-1]\right\}k_V(x,y,z,T)V\,(x,y,z,t)d\,z\,d\,y\,d\,x+\frac{1}{\pi^3}\sum_{n=1}^{N}\frac{a_{n\Phi V}}{n^3}\times$$

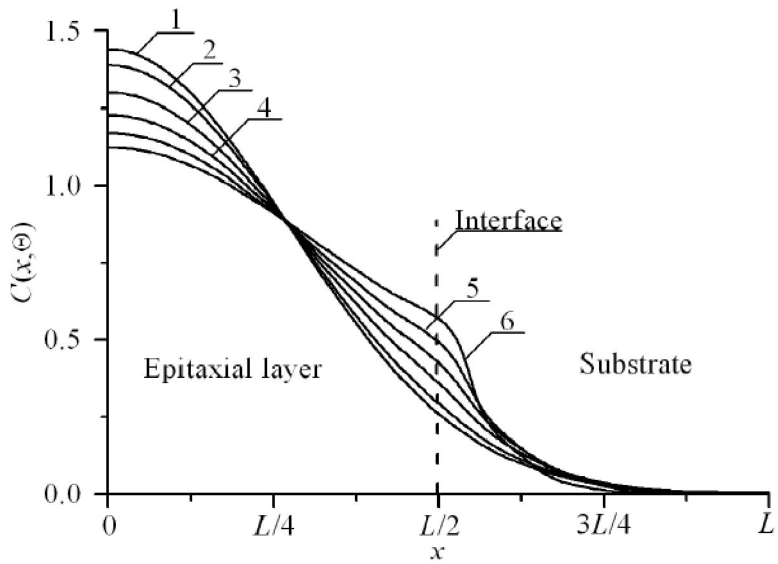

Figure 2a : Distributions of concentration of infused dopant in heterostructure from Figs. 1 and 2 in direction, which is perpendicular to interface between epitaxial layer substrate. Increasing of number of curve corresponds to increasing of difference between values of dopant diffusion coefficient in layers of heterostructure under condition, when value of dopant diffusion coefficient in epitaxial layer is larger, than value of dopant diffusion coefficient in substrate

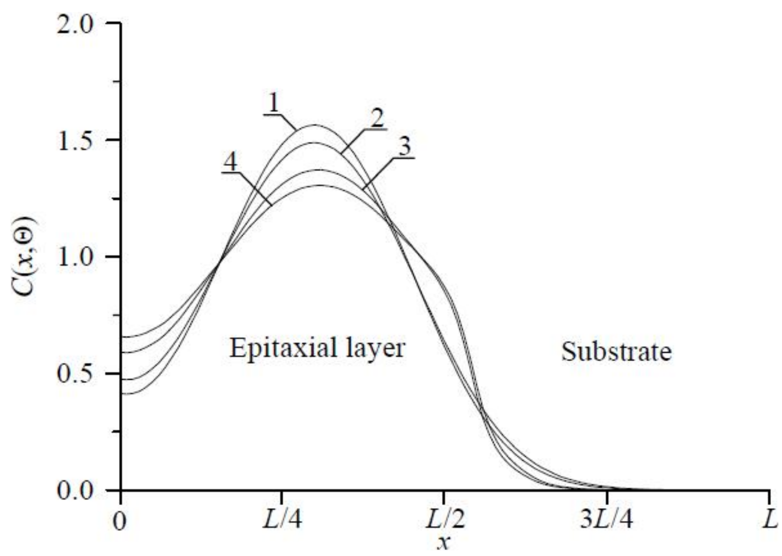

Figure 2b : Distributions of concentration of implanted dopant in heterostructure from Figs. 1 and 2 in direction, which is perpendicular to interface between epitaxial layer substrate. Curves 1 and 3 corresponds to annealing time $\Theta = 0.0048(L_x^2+L_y^2+L_z^2)/D_0$. Curves 2 and 4 corresponds to annealing time $\Theta = 0.0057(L_x^2+L_y^2+L_z^2)/D_0$. Curves 1 and 2 corresponds to homogenous sample. Curves 3 and 4 corresponds to heterostructure under condition, when value of dopant diffusion coefficient in epitaxial layer is larger, than value of dopant diffusion coefficient in substrate

$$\times\int_0^t e_{n\Phi V}(\tau)\int_0^{L_x}\left\{x\,s_n(x)+\frac{L_x}{2\pi n}\left[c_n(x)-1\right]\right\}\int_0^{L_y}\left\{y\,s_n(y)+\frac{L_y}{2\pi n}\left[c_n(y)-1\right]\right\}\int_0^{L_z}\left\{\frac{L_z}{2\pi n}\left[c_n(z)-1\right]+\right.$$

$$\left.+\,z\,s_n(z)\right\}f_{\Phi V}(x,y,z)\,d\,z\,d\,y\,d\,x\,.$$

DISCUSSION

In this section we analyzed the spatio-temporal distribution of concentration of dopant in the considered heterostructure during annealing. Figures 2 shows spatial distributions of concentrations of dopants infused (Figure 2a) or implanted (Figure 2b) in epitaxial layer. Value of annealing time is equal for all distributions framework every Figure 2a and 2b. Increasing of number of curves corresponds to increasing of difference between values

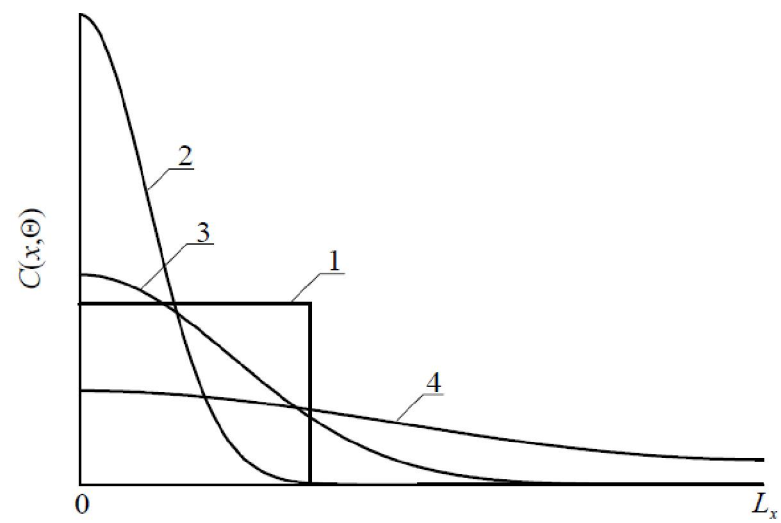

Figure 3a : Spatial distributions of dopant in heterostructure after dopant infusion. Curve 1 is idealized distribution of dopant. Curves 2-4 are real distributions of dopant for different values of annealing time. Increasing of number of curve corresponds to increasing of annealing time

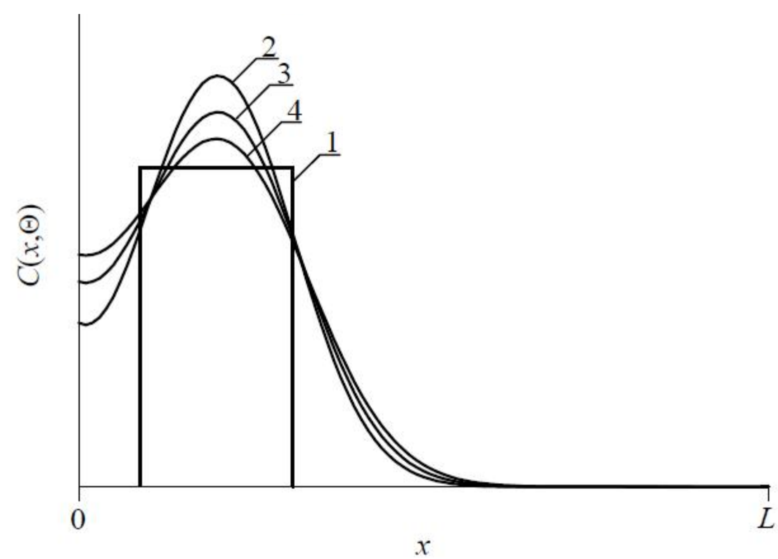

Figure 3b : Spatial distributions of dopant in heterostructure after ion implantation. Curve 1 is idealized distribution of dopant. Curves 2-4 are real distributions of dopant for different values of annealing time. Increasing of number of curve corresponds to increasing of annealing time

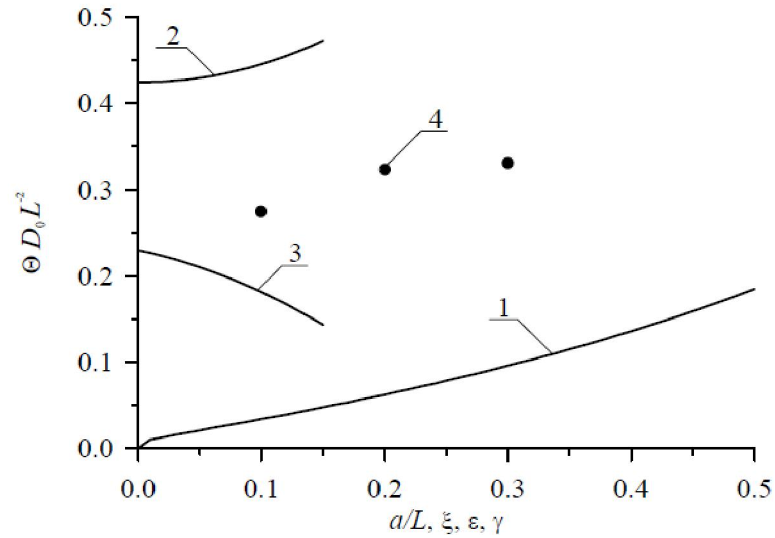

Figure 4a : Dependences of dimensionless optimal annealing time for doping by diffusion, which have been obtained by minimization of mean-squared error, on several parameters. Curve 1 is the dependence of dimensionless optimal annealing time on the relation a/L and ξ = γ = 0 for equal to each other values of dopant diffusion coefficient in all parts of heterostructure. Curve 2 is the dependence of dimensionless optimal annealing time on value of parameter ε for a/L=1/2 and ξ = γ = 0. Curve 3 is the dependence of dimensionless optimal annealing time on value of parameter ξ for a/L =1/2 and ε = γ = 0. Curve 4 is the dependence of dimensionless optimal annealing time on value of parameter γ for a/L=1/2 and ε = ξ = 0

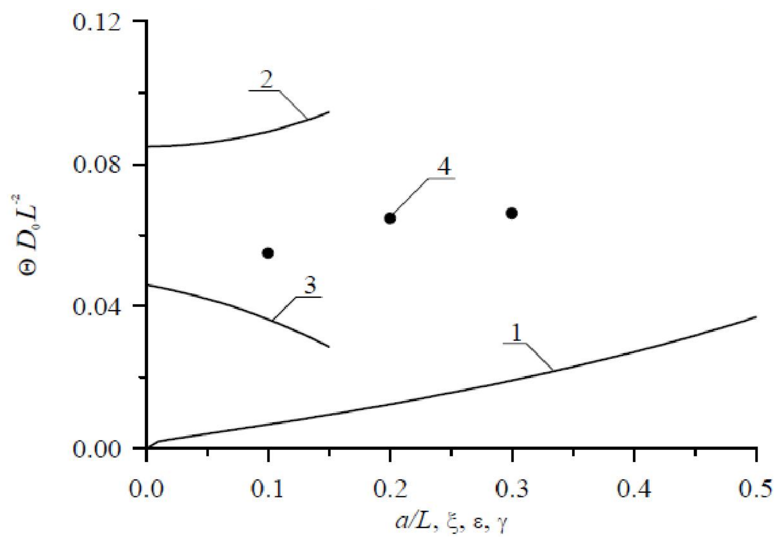

Figure 4b : Dependences of dimensionless optimal annealing time for doping by ion implantation, which have been obtained by minimization of mean-squared error, on several parameters. Curve 1 is the dependence of dimensionless optimal annealing time on the relation a/L and ξ = γ = 0 for equal to each other values of dopant diffusion coefficient in all parts of heterostructure. Curve 2 is the dependence of dimensionless optimal annealing time on value of parameter ε for a/L=1/2 and ξ = γ = 0. Curve 3 is the dependence of dimensionless optimal annealing time on value of parameter ξ for a/L =1/2 and = γ = 0. Curve 4 is the dependence of dimensionless optimal annealing time on value of parameter γ for a/L=1/2 and ε = ξ = 0

of dopant diffusion coefficients in layers of heterostructure. The figures show that presents of interface between layers of heterostructure gives us possibility to increase absolute value of gradient of concentration of dopant in direction, which is perpendicular to the interface. We obtain increasing of absolute value of the gradient in neighborhood of the interface. Due to the increasing one can obtain decreasing dimensions of transistors, which have been used in the element "OR". At the same time with increasing of the gradient homogeneity of concentration of dopant in enriched area increases.

To choose annealing time it should be accounted decreasing of absolute value of gradient of concentration of dopant in neighborhood of interface between substrate and epitaxial layer with increasing of annealing time. Decreasing of value of annealing time leads to decreasing of homogeneity of concentration of dopant in enriched area (see Figure 3a for diffusion doping of materials and Figure 3b for ion doping of materials). Let us determine compromise value of annealing time framework recently introduced criteria[17-22]. Framework the criteria we approximate real distributions of concentration of dopant by ideal rectangle distribution ψ (x,y,z). Farther we determine compromise value of annealing time by minimization of the mean-squared error

$$U=\frac{1}{L_xL_yL_z}\int_0^{L_x}\int_0^{L_y}\int_0^{L_z}\left[C\left(x,y,z,\Theta\right)-\psi\left(x,y,z\right)\right]d\,z\,d\,y\,d\,x\,. \quad (8)$$

Dependences of optimal annealing time are presented on Figs. 4 for diffusion and ion types of doping, respectively. It should be noted, that it is necessary to anneal radiation defects after ion implantation. One could find spreading of concentration of distribution of dopant during this annealing. In the ideal case distribution of dopant achieves appropriate interfaces between materials of heterostructure during annealing of radiation defects. If dopant did not achieves any interfaces during annealing of radiation defects, it is practicably to additionally anneal the dopant. In this situation optimal value of additional annealing time of implanted dopant is smaller, than annealing time of infused dopant. At the same time ion type of doping gives us possibility to decrease mismatch-induced stress in heterostructure[23].

CONCLUSION

In this paper we model redistribution of infused and implanted dopants during ma-nufacture logical elements "OR" based on field-effect heterotransistors. Several recommendations to optimize manufacture the heterotransistors have been formulated. Analytical approach to model diffusion and ion types of doping with account concurrent changing of parameters in space and time has been introduced. At the same time the approach gives us possibility to take into account nonlinearity of doping processes.

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