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OPTIMIZATION OF TECHNOLOGICAL PROCESS TO DECREASE DIMENSIONS OF CIRCUITS XOR, MANUFECTURED BASED ON FIELD-EFFECT HETEROTRANSISTORS

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ABSTRACT

The paper describes an approach of increasing of integration rate of elements of integrated circuits. The approach has been illustrated by example of manufacturing of a circuit XOR. Framework the approach one should manufacture a heterostructure with specific configuration. After that several special areas of the heterostructure should be doped by diffusion and/or ion implantation and optimization of annealing of dopant and/or radiation defects. We analyzed redistribution of dopant with account redistribution of radiation defects to formulate recommendations to decrease dimensions of integrated circuits by using analytical approaches of modeling of technological process.

KEYWORDS

Circuits XOR; increasing of density of elements; optimization of technological process.

1. INTRODUCTION

One of intensively solving problems of solid state electronics is improvement of frequency characteristics of electronic devices and their reliability. Another intensively solving problem is increasing of integration rate of integrated circuits with decreasing of their dimensions [1-9]. To solve these problems they were used searching materials with higher values of charge carriers motilities, development new and elaboration existing technological approaches [1-14]. In the present paper we consider circuit XOR from [15]. Based on recently considered approaches [16-23] we consider an approach to decrease dimensions of the circuit. The approach based on manufacturing a heterostructure, which consist of a substrate and an epitaxial layer. The epitaxial layer manufactured with several sections. To manufacture these sections another materials have been used. These sections have been doped by diffusion or ion implantation. The doping gives a possibility to generate another type of conductivity (*p* or *n*). After finishing of manufacturing of the circuit XOR these sections will be used by sources, drains and gates (see Fig. 1). Dopant and radiation defects should be annealed after finishing the dopant diffusion and the ion implantation. Our aim framework the paper is analysis of redistribution of dopant and redistribution of radiation defects to prognosis technological process. The accompanying aim of the present paper is development of analytical approach for prognosis technological processes with account all required influenced factors.

2. METHOD OF SOLUTION

We solve our aim by calculation and analysis distribution of concentrations of dopants in space and time. The required distribution has been determined by solving the second Fick's law in the following form [24,25]

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

Boundary and initial conditions for the equations are

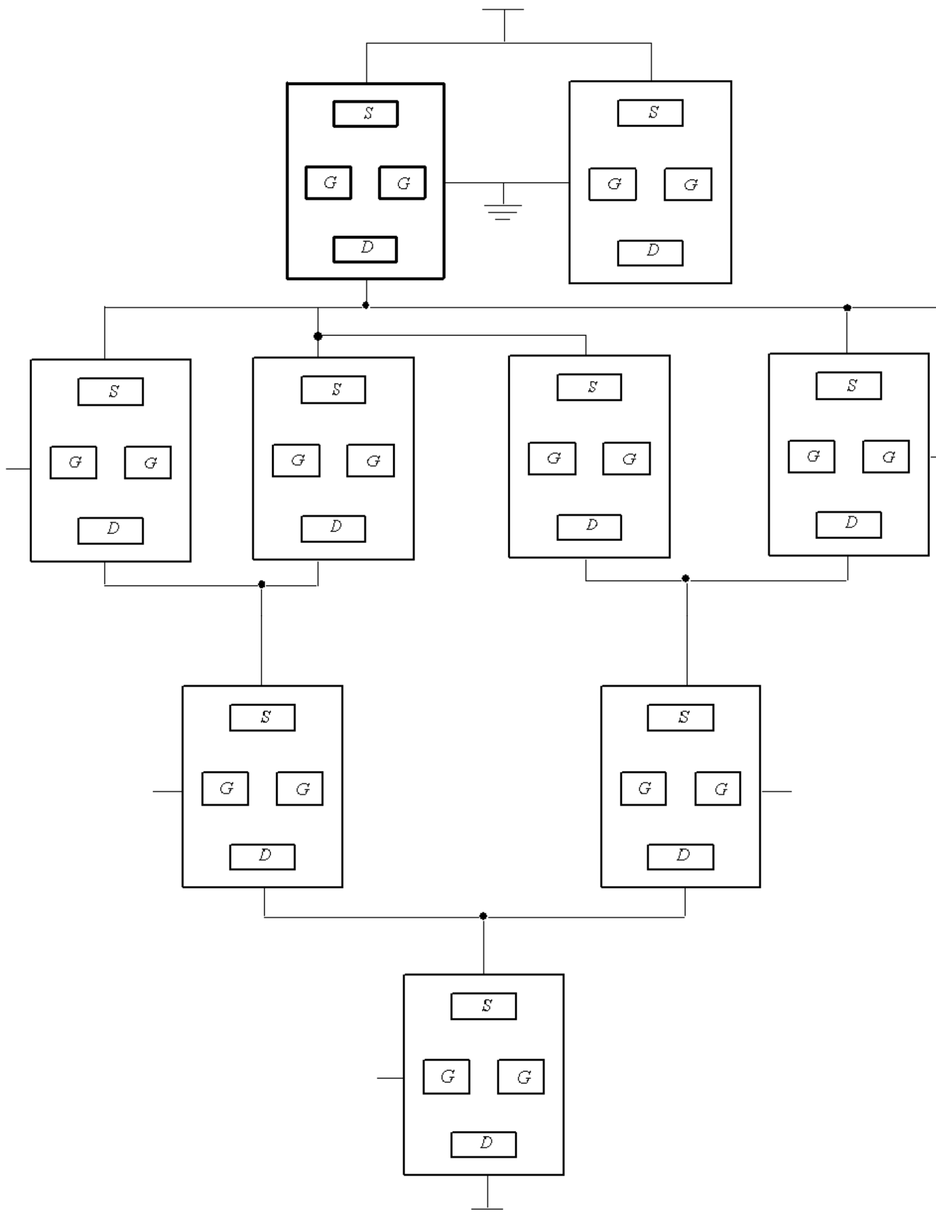

Fig. 1. Structure of epitaxial layer. View from top

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

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

Here the function $C(x,y,z,t)$ describes the distribution of concentration of dopant in space and time. D_C describes distribution the dopant diffusion coefficient in space and as a function of temperature of annealing. Dopant diffusion coefficient will be changed with changing of materials of heterostructure, heating and cooling of heterostructure during annealing of dopant or radiation defects (with account Arrhenius law). Dependences of dopant diffusion coefficient on coordinate in heterostructure, temperature of annealing and concentrations of dopant and radiation defects could be written as [26-28]

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

Here function $D_L(x,y,z,T)$ describes dependences of dopant diffusion coefficient on coordinate and temperature of annealing T. Function $P(x,y,z,T)$ describes the same dependences of the limit of solubility of dopant. The parameter γ is integer and usually could be varying in the following interval $\gamma\in[1,3]$. The parameter describes quantity of charged defects, which interacting (in average) with each atom of dopant. Ref.[26] describes more detailed information about dependence of dopant diffusion coefficient on concentration of dopant. Spatio-temporal distribution of concentration of radiation vacancies described by the function $V(x,y,z,t)$. The equilibrium distribution of concentration of vacancies has been denoted as V^*. It is known, that doping of materials by diffusion did not leads to radiation damage of materials. In this situation $\zeta_1=\zeta_2=0$. We determine spatio-temporal distributions of concentrations of radiation defects by solving the following system of equations [27,28]

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

$$\times I^2(x,y,z,t)+\frac{\partial}{\partial z}\left[D_I(x,y,z,T)\frac{\partial I(x,y,z,t)}{\partial z}\right]-k_{I,V}(x,y,z,T)\,I(x,y,z,t)\,V(x,y,z,t) \quad (4)$$

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

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

Boundary and initial conditions for these equations are

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

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

Here $\rho=I,V$. We denote spatio-temporal distribution of concentration of radiation interstitials as $I(x,y,z,t)$. Dependences of the diffusion coefficients of point radiation defects on coordinate and temperature have been denoted as $D_\rho(x,y,z,T)$. The quadric on concentrations terms of Eqs. (4) describes generation divacancies and diinterstitials. Parameter of recombination of point radiation defects and parameters of generation of simplest complexes of point radiation defects have been denoted as the following functions $k_{I,V}(x,y,z,T)$, $k_{I,I}(x,y,z,T)$ and $k_{V,V}(x,y,z,T)$, respectively.

Now let us calculate distributions of concentrations of divacancies $\Phi_V(x,y,z,t)$ and diinterstitials $\Phi_I(x,y,z,t)$ in space and time by solving the following system of equations [27,28]

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

Boundary and initial conditions for these equations are

$$\left.\frac{\partial\Phi_\rho(x,y,z,t)}{\partial x}\right|_{x=0}=0,\ \left.\frac{\partial\Phi_\rho(x,y,z,t)}{\partial x}\right|_{x=L_x}=0,\ \left.\frac{\partial\Phi_\rho(x,y,z,t)}{\partial y}\right|_{y=0}=0,\ \left.\frac{\partial\Phi_\rho(x,y,z,t)}{\partial y}\right|_{y=L_y}=0,$$
$$\left.\frac{\partial\Phi_\rho(x,y,z,t)}{\partial z}\right|_{z=0}=0,\ \left.\frac{\partial\Phi_\rho(x,y,z,t)}{\partial z}\right|_{z=L_z}=0,\ \Phi_I(x,y,z,0)=f_{\Phi I}(x,y,z),\ \Phi_V(x,y,z,0)=f_{\Phi V}(x,y,z). \tag{7}$$

The functions $D_{\Phi\rho}(x,y,z,T)$ describe dependences of the diffusion coefficients of the above complexes of radiation defects on coordinate and temperature. The functions $k_I(x,y,z,T)$ and $k_V(x,y,z,T)$ describe the parameters of decay of these complexes on coordinate and temperature.

To describe physical processes they are usually solving nonlinear equations with space and time varying coefficients. In this situation only several limiting cases have been analyzed [29-32]. One way to solve the problem is solving the Eqs. (1), (4), (6) by the Bubnov-Galerkin approach [33] after appropriate transformation of these transformation. To determine the spatio-temporal distribution of concentration of dopant we transform the Eq.(1) to the following integro- differential form

$$\frac{x\,y\,z}{L_xL_yL_z}\int\limits_{L_x}^{x}\int\limits_{L_y}^{y}\int\limits_{L_z}^{z}C(u,v,w,t)\,d\,w\,d\,v\,d\,u=\int\limits_0^t\int\limits_{L_y}^{y}\int\limits_{L_z}^{z}D_L(x,v,w,T)\left[1+\varsigma_1\frac{V(x,v,w,\tau)}{V^*}+\varsigma_2\frac{V^2(x,v,w,\tau)}{(V^*)^2}\right]\times$$

$$\times\left[1+\xi\frac{C^{\gamma}(x,v,w,\tau)}{P^{\gamma}(x,v,w,T)}\right]\frac{\partial\, C(x,v,w,\tau)}{\partial\, x}\,d\,\tau\frac{y\,z}{L_y L_z}+\int\limits_0^t\int\limits_{L_x}^x\int\limits_{L_z}^z D_L(u,y,w,T)\left[1+\xi\frac{C^{\gamma}(u,y,w,\tau)}{P^{\gamma}(x,y,z,T)}\right]\times$$

$$\times\left[1+\varsigma_1\frac{V(u,y,w,\tau)}{V^*}+\varsigma_2\frac{V^2(u,y,w,\tau)}{(V^*)^2}\right]\frac{\partial\, C(u,y,w,\tau)}{\partial\, y}\,d\,\tau\frac{x\,z}{L_x L_z}+\int\limits_0^t\int\limits_{L_x}^x\int\limits_{L_y}^y D_L(u,v,z,T)\times$$

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

$$+\frac{x\,y\,z}{L_x L_y L_z}\int\limits_{L_x}^x\int\limits_{L_y}^y\int\limits_{L_z}^z f(u,v,w)\,d\,w\,d\,v\,d\,u\,. \qquad (1a)$$

Now let us determine solution of Eq.($1a$) by Bubnov-Galerkin approach [33]. To use the approach we consider solution of the Eq.($1a$) as the following series

$$C_0(x,y,z,t)=\sum_{n=0}^{N}a_{nC}\,c_n(x)\,c_n(y)\,c_n(z)\,e_{nC}(t).$$

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

$$\frac{x\,y\,z}{\pi^2}\sum_{n=1}^{N}\frac{a_C}{n^3}s_n(x)\,s_n(y)\,s_n(z)\,e_{nC}(t)=-\frac{y\,z}{L_y L_z}\int\limits_0^t\int\limits_{L_y}^y\int\limits_{L_z}^z\left\{1+\left[\sum_{n=1}^{N}a_{nC}\,c_n(x)\,c_n(v)\,c_n(w)\,e_{nC}(\tau)\right]^{\gamma}\times\right.$$

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

$$\times n\,c_n(w)\,e_{nC}(\tau)d\,\tau-\frac{x\,z}{L_x L_z}\int\limits_0^t\int\limits_{L_x}^x\int\limits_{L_z}^z\left\{1+\left[\sum_{m=1}^{N}a_{mC}\,c_m(u)\,c_m(y)\,c_m(w)\,e_{mC}(\tau)\right]^{\gamma}\frac{\xi}{P^{\gamma}(u,y,w,T)}\right\}\times$$

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

$$\times a_{nC}-\frac{x\,y}{L_x L_y}\int\limits_0^t\int\limits_{L_x}^x\int\limits_{L_y}^y D_L(u,v,z,T)\left\{1+\frac{\xi}{P^{\gamma}(u,v,z,T)}\left[\sum_{n=1}^{N}a_{nC}\,c_n(u)\,c_n(v)\,c_n(z)\,e_{nC}(\tau)\right]^{\gamma}\right\}\times$$

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

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

where $s_n(\chi)=sin(\pi n\chi/L_\chi)$. We used condition of orthogonality to determine coefficients a_n in the considered series. The coefficients a_n could be calculated for any quantity of terms N. In the common case the relations could be written as

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

where $\alpha_n=\frac{\xi L_yL_z}{2\pi^2n}\int_0^t e_{nC}(\tau)\int_0^{L_x}s_n(2x)\int_0^{L_y}c_n(y)\int_0^{L_z}c_n(z)\left[1+\varsigma_1\frac{V(x,y,z,\tau)}{V^*}+\varsigma_2\frac{V^2(x,y,z,\tau)}{(V^*)^2}\right]\times$

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

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

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

$$\times\int_0^t e_{nC}(\tau)\int_0^{L_x}c_n(x)\int_0^{L_y}c_n(y)\int_0^{L_z}s_n(2z)\frac{D_L(x,y,z,T)}{P(x,y,z,T)}\left[1+\varsigma_1\frac{V(x,y,z,\tau)}{V^*}+\varsigma_2\frac{V^2(x,y,z,\tau)}{(V^*)^2}\right]\times$$

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

$$\times\int_0^{L_x}s_n(2x)\int_0^{L_y}c_n(y)\left\{y\,s_n(y)+\frac{L_y}{\pi n}\left[c_n(y)-1\right]\right\}\int_0^{L_z}c_n(z)\left[1+\varsigma_1\frac{V(x,y,z,\tau)}{V^*}+\varsigma_2\frac{V^2(x,y,z,\tau)}{(V^*)^2}\right]\times$$

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

$$\times\left\{x\,s_n(x)+\frac{L_x}{\pi n}\left[c_n(x)-1\right]\right\}\int_0^{L_z}D_L(x,y,z,T)\,c_n(z)\left[1+\varsigma_1\frac{V(x,y,z,\tau)}{V^*}+\varsigma_2\frac{V^2(x,y,z,\tau)}{(V^*)^2}\right]\times$$

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

$$\times c_n(x)\int_0^{L_y}\left\{y\,s_n(y)+\frac{L_y}{\pi n}\left[c_n(y)-1\right]\right\}\int_0^{L_z}D_L(x,y,z,T)\left[1+\varsigma_1\frac{V(x,y,z,\tau)}{V^*}+\varsigma_2\frac{V^2(x,y,z,\tau)}{(V^*)^2}\right]\times$$

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

The same approach could be used for calculation parameters a_n for different values of parameter γ. However the relations are bulky and will not be presented in the paper. Advantage of the approach is absent of necessity to join dopant concentration on interfaces of heterostructure.

The same Bubnov-Galerkin approach has been used for solution the Eqs.(4). Previously we transform the differential equations to the following integro- differential form

$$\frac{x\,y\,z}{L_xL_yL_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}I(u,v,w,t)\,d\,w\,d\,v\,d\,u=\frac{y\,z}{L_yL_z}\int_0^t\int_{L_y}^{y}\int_{L_z}^{z}D_I(x,v,w,T)\frac{\partial I(x,v,w,\tau)}{\partial x}d\,w\,d\,v\,d\,\tau+$$

$$+\frac{x\,z}{L_xL_z}\int_0^t\int_{L_x}^{x}\int_{L_z}^{z}D_I(u,y,w,T)\frac{\partial I(u,y,w,\tau)}{\partial x}d\,w\,d\,u\,d\,\tau-\frac{x\,y\,z}{L_xL_yL_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}k_{I,V}(u,v,w,T)\,I(u,v,w,t)\times$$

$$\times\ V(u,v,w,t)\,d\,w\,d\,v\,d\,u+\frac{x\,y}{L_xL_y}\int_0^t\int_{L_x}^{x}\int_{L_y}^{y}\frac{\partial I(u,v,z,\tau)}{\partial z}D_I(u,v,z,T)\,d\,v\,d\,u\,d\,\tau-\frac{x\,y\,z}{L_xL_yL_z}\times$$

$$\times\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}k_{I,I}(u,v,w,T)\,I^2(u,v,w,t)\,d\,w\,d\,v\,d\,u+\frac{x\,y\,z}{L_xL_yL_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}f_I(u,v,w)\,d\,w\,d\,v\,d\,u\qquad(4a)$$

$$\frac{x\,y\,z}{L_xL_yL_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}V(u,v,w,t)\,d\,w\,d\,v\,d\,u=\frac{y\,z}{L_yL_z}\int_0^t\int_{L_y}^{y}\int_{L_z}^{z}D_V(x,v,w,T)\frac{\partial V(x,v,w,\tau)}{\partial x}d\,w\,d\,v\,d\,\tau+$$

$$+\frac{x\,z}{L_xL_z}\int_0^t\int_{L_x}^{x}\int_{L_z}^{z}D_V(u,y,w,T)\frac{\partial V(u,y,w,\tau)}{\partial x}d\,w\,d\,u\,d\,\tau+\frac{x\,y}{L_xL_y}\int_0^t\int_{L_x}^{x}\int_{L_y}^{y}\frac{\partial V(u,v,z,\tau)}{\partial z}\times$$

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

$$-\frac{x\,y\,z}{L_xL_yL_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}k_{V,V}(u,v,w,T)\,V^2(u,v,w,t)\,d\,w\,d\,v\,d\,u+\frac{x\,y\,z}{L_xL_yL_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z}f_V(u,v,w)\,d\,w\,d\,v\,d\,u\,.$$

We determine spatio-temporal distributions of concentrations of point defects as the same series

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

Parameters $a_{n\rho}$ should be determined in future. Substitution of the series into Eqs.(4a) leads to the following results

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

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

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

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

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

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

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

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

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

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

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

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

We used orthogonality condition of functions of the considered series framework the heterostructure to calculate coefficients $a_{n\rho}$. The coefficients a_n could be calculated for any quantity of terms N. In the common case equations for the required coefficients could be written as

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\times d\,y\,d\,x\,d\,\tau-\frac{L_x^2L_y^2L_z^2}{\pi^5n^6}e_{n\rho}(t),\ \chi_{nIV}=\int\limits_0^{L_x}\left\{x\,s_n(x)+\frac{L_x}{\pi n}\left[c_n(x)-1\right]\right\}\int\limits_0^{L_y}\Big\{L_y+\frac{L_y}{2\pi n}\left[c_n(2y)-1\right]+$$

$$+y\,s_n(2y)\Big\}\int\limits_0^{L_z}k_{I,V}(x,y,z,T)\left\{L_z+z\,s_n(2z)+\frac{L_z}{2\pi n}\left[c_n(2z)-1\right]\right\}d\,z\,d\,y\,d\,x\,e_{nI}(t)\,e_{nV}(t),$$

$$\lambda_{n\rho}=\int\limits_0^{L_x}\left\{x\,s_n(x)+\frac{L_x}{\pi n}\left[c_n(x)-1\right]\right\}\int\limits_0^{L_y}\left\{y\,s_n(y)+\frac{L_y}{\pi n}\left[c_n(y)-1\right]\right\}\int\limits_0^{L_z}\left\{z\,s_n(z)+\frac{L_z}{\pi n}\left[c_n(z)-1\right]\right\}\times$$

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

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

$$\times\gamma_{nV}\delta_{nI}-\delta_{nV}\chi_{nI}\lambda_{nI},\ y=\sqrt[3]{\sqrt{q^2+p^3}-q}-\sqrt[3]{\sqrt{q^2+p^3}+q}-\frac{b_3}{3b_4},\ p=\frac{3b_2b_4-b_3^2}{9b_4^2},$$

$$q=\left(2b_3^3-9b_2b_3+27b_1b_4^2\right)/54b_4^3.$$

We determine distributions of concentrations of simplest complexes of radiation defects in space and time as the following functional series

$$\Phi_{\rho0}(x,y,z,t)=\sum_{n=1}^{N}a_{n\Phi\rho}\,c_n(x)\,c_n(y)\,c_n(z)\,e_{n\rho}(t).$$

Here $a_{n\Phi\rho}$ are the coefficients, which should be determined. Let us previously transform the Eqs. (6) to the following integro-differential form

$$\frac{x\,y\,z}{L_xL_yL_z}\int\limits_{L_x}^{x}\int\limits_{L_y}^{y}\int\limits_{L_z}^{z}\Phi_I(u,v,w,t)\,d\,w\,d\,v\,d\,u=\int\limits_0^t\int\limits_{L_y}^{y}\int\limits_{L_z}^{z}D_{\Phi I}(x,v,w,T)\frac{\partial\,\Phi_I(x,v,w,\tau)}{\partial x}d\,w\,d\,v\,d\,\tau\times$$

$$\times\frac{y\,z}{L_yL_z}+\frac{x\,z}{L_xL_z}\int\limits_0^t\int\limits_{L_x}^{x}\int\limits_{L_z}^{z}D_{\Phi I}(u,y,w,T)\frac{\partial\,\Phi_I(u,y,w,\tau)}{\partial y}d\,w\,d\,u\,d\,\tau+\frac{x\,y}{L_xL_y}\int\limits_0^t\int\limits_{L_x}^{x}\int\limits_{L_y}^{y}D_{\Phi I}(u,v,z,T)\times$$

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

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

$$\frac{x\,y\,z}{L_xL_yL_z}\int\limits_{L_x}^{x}\int\limits_{L_y}^{y}\int\limits_{L_z}^{z}\Phi_V(u,v,w,t)\,d\,w\,d\,v\,d\,u=\int\limits_0^t\int\limits_{L_y}^{y}\int\limits_{L_z}^{z}D_{\Phi V}(x,v,w,T)\frac{\partial\,\Phi_V(x,v,w,\tau)}{\partial x}d\,w\,d\,v\,d\,\tau\times$$

$$\times\frac{y\,z}{L_yL_z}+\frac{x\,z}{L_xL_z}\int\limits_0^t\int\limits_{L_x}^{x}\int\limits_{L_z}^{z}D_{\Phi V}(u,y,w,T)\frac{\partial\,\Phi_V(u,y,w,\tau)}{\partial y}d\,w\,d\,u\,d\,\tau+\frac{x\,y}{L_xL_y}\int\limits_0^t\int\limits_{L_x}^{x}\int\limits_{L_y}^{y}D_{\Phi V}(u,v,z,T)\times$$

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

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

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

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

$$\times D_{\Phi I}(x,v,w,T)d\,w\,d\,v\,d\,\tau-\frac{x\,z\,\pi}{L_xL_yL_z}\sum_{n=1}^{N}a_{n\Phi I}\int\limits_0^t\int\limits_{L_x}^{x}\int\limits_{L_z}^{z}c_n(u)c_n(w)\,D_{\Phi I}(u,v,w,T)\,d\,w\,d\,u\,d\,\tau\times$$

$$\times n\,s_n(y)e_{n\Phi I}(t)-\frac{x\,y\,\pi}{L_xL_yL_z}\sum_{n=1}^{N}n\,a_{n\Phi I}\,s_n(z)e_{n\Phi I}(t)\int\limits_0^t\int\limits_{L_x}^{x}\int\limits_{L_y}^{y}c_n(u)c_n(v)\,D_{\Phi I}(u,v,z,T)\,d\,v\,d\,u\,d\,\tau+$$

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

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

$$-x\,y\,z\sum_{n=1}^{N}\frac{a_{n\Phi V}}{\pi^3n^3}s_n(x)\,s_n(y)\,s_n(z)\,e_{nV}(t)=-\frac{y\,z\,\pi}{L_xL_yL_z}\sum_{n=1}^{N}n\,a_{n\Phi V}\,s_n(x)e_{nV}(t)\int\limits_0^t\int\limits_{L_y}^{y}\int\limits_{L_z}^{z}c_n(v)c_n(w)\times$$

$$\times D_{\Phi V}(x,v,w,T)\,d\,w\,d\,v\,d\,\tau-\frac{x\,z\,\pi}{L_xL_yL_z}\sum_{n=1}^{N}n\int\limits_0^t\int\limits_{L_x}^{x}\int\limits_{L_z}^{z}c_n(u)c_n(w)\,D_{\Phi V}(u,v,w,T)\,d\,w\,d\,u\,d\,\tau\times$$

$$\times a_{n\Phi V}\,s_n(y)e_{n\Phi V}(t)-\frac{x\,y\,\pi}{L_xL_yL_z}\sum_{n=1}^{N}n\,s_n(z)e_{n\Phi V}(t)\int\limits_0^t\int\limits_{L_x}^{x}\int\limits_{L_y}^{y}c_n(u)c_n(v)\,D_{\Phi V}(u,v,z,T)\,d\,v\,d\,u\,d\,\tau\times$$

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

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

We used orthogonality condition of functions of the considered series framework the heterostructure to calculate coefficients $a_{n\Phi\rho}$. The coefficients $a_{n\Phi\rho}$ could be calculated for any quantity of terms *N*. In the common case equations for the required coefficients could be written as

$$-\frac{L_x^2L_y^2L_z^2}{\pi^5}\sum_{n=1}^{N}\frac{a_{n\Phi I}}{n^6}e_{n\Phi I}(t)=-\frac{1}{2\pi\,L_x}\sum_{n=1}^{N}\int\limits_0^t\int\limits_0^{L_x}[1-c_n(2x)]\int\limits_0^{L_y}\left\{L_y+y\,s_n(2y)+\frac{L_y}{2\pi\,n}[c_n(2y)-1]\right\}\times$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$+x\,s_n(x)\Big\}\int\limits_0^{L_y}\left\{y\,s_n(y)+\frac{L_y}{2\pi n}[c_n(y)-1]\right\}\int\limits_0^{L_z}V^2(x,y,z,t)\,k_{V,V}(x,y,z,T)\left\{\frac{L_z}{2\pi n}[c_n(z)-1]+\right.$$

$$\left.+z\,s_n(z)\right\}d\,z\,d\,y\,d\,x-\frac{1}{\pi^3}\sum_{n=1}^{N}\frac{a_{n\Phi V}}{n^3}\int\limits_0^t e_{n\Phi V}(\tau)\int\limits_0^{L_x}\left\{x\,s_n(x)+\frac{L_x}{2\pi n}[c_n(x)-1]\right\}\int\limits_0^{L_y}\left\{\frac{L_y}{2\pi n}[c_n(y)-1]+\right.$$

$$\left.+y\,s_n(y)\right\}\int\limits_0^{L_z}\left\{z\,s_n(z)+\frac{L_z}{2\pi n}[c_n(z)-1]\right\}k_V(x,y,z,T)V\,(x,y,z,t)d\,z\,d\,y\,d\,x+\frac{1}{\pi^3}\sum_{n=1}^{N}\frac{a_{n\Phi V}}{n^3}\times$$

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

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

3. Discussion

In this section we analyzed redistribution of dopant with account redistribution of radiation defects. The analysis shown, that presents of interface between materials of heterostructure gives a possibility to increase absolute value of gradient of concentration of dopant outside of enriched are by the dopant (see Figs. 2 and 3). At the same time homogeneity of concentration of dopant in enriched area increases (see Figs. 2 and 3). The effects could be find, when dopant diffusion coefficient in the doped area is larger, than in the nearest areas. Otherwise absolute value of gradient of concentration of dopant decreases outside enriched by the dopant area (see Fig. 4). However the decreasing could be partially or fully compensated by using high doping of materials. The high doping leads to significant nonlinearity of diffusion of dopant. To increase compactness of the considered circuits XOR it is attracted an interest the first relation between values of dopant diffusion coefficient.

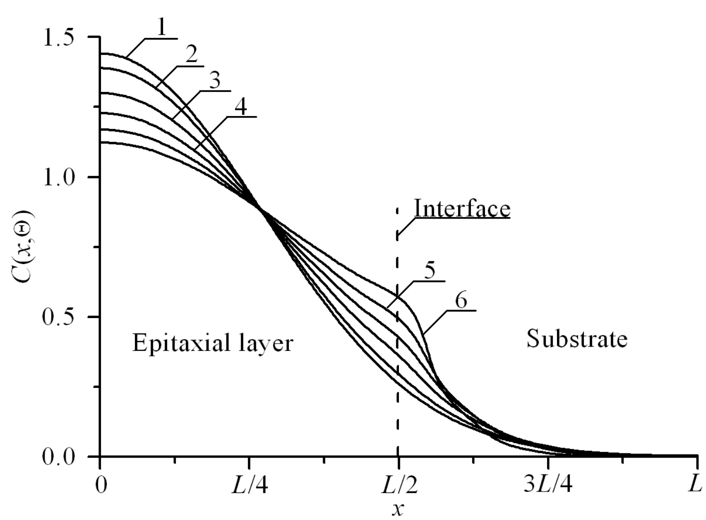

Fig.2*a*. Spatial distributions of infused dopant concentration in the considered heterostructure. The considered direction perpendicular to the interface between epitaxial layer substrate. Difference between values of dopant diffusion coefficient in layers of heterostructure increases with increasing of number of curves

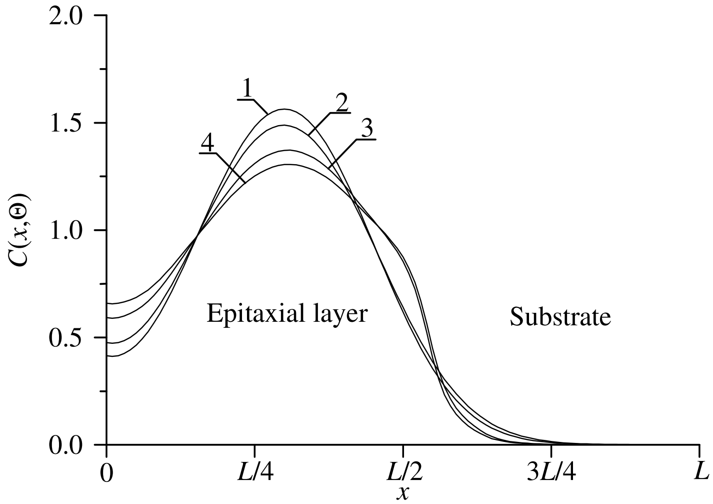

Fig.2*b*. Spatial distributions of infused dopant concentration in the considered heterostructure. Curves 1 and 3 corresponds to annealing time $\Theta=0.0048(L_x^2+L_y^2+L_z^2)/D_0$. Curves 2 and 4 corresponds to annealing time $\Theta=0.0057(L_x^2+L_y^2+L_z^2)/D_0$. Curves 1 and 2 corresponds to homogenous sample. Curves 3 and 4 corresponds to the considered heterostructure. Difference between values of dopant diffusion coefficient in layers of heterostructure increases with increasing of number of curves

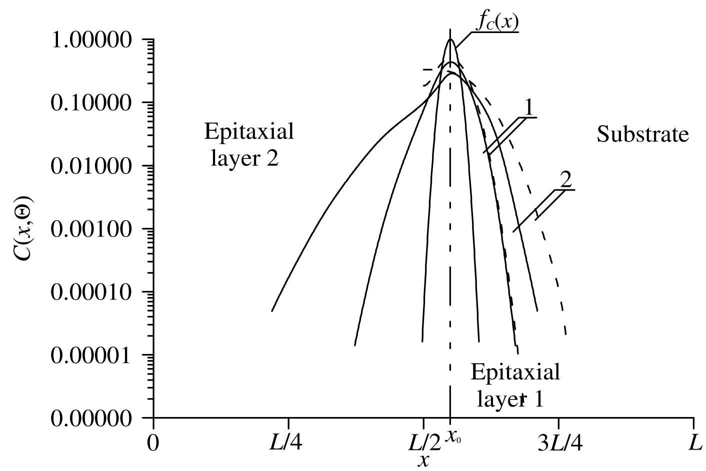

Fig.3. Implanted dopant distributions in heterostructure in heterostructure with two epitaxial layers (solid lines) and with one epitaxial layer (dushed lines) for different values of annealing time. Difference between values of dopant diffusion coefficient in layers of heterostructure increases with increasing of number of curves

Increasing of annealing time leads to acceleration of diffusion. In this situation one can find increasing quantity of dopant in materials near doped sections. If annealing time is small, the dopant can not achieves nearest interface between layers of heterostructure. These effects are shown by Figs. 5 and 6. We used recently introduced criterion [16-23] to estimate compromise value of annealing time. Framework the criterion we approximate real distribution of concentration of dopant by idealized step-wise distribution $\psi(x,y,z)$, which would be better to use for minimization dimensions of elements of the considered circuit XOR [19-26]. Farther the required compromise annealing time has been calculated by minimization the following mean-squared error

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

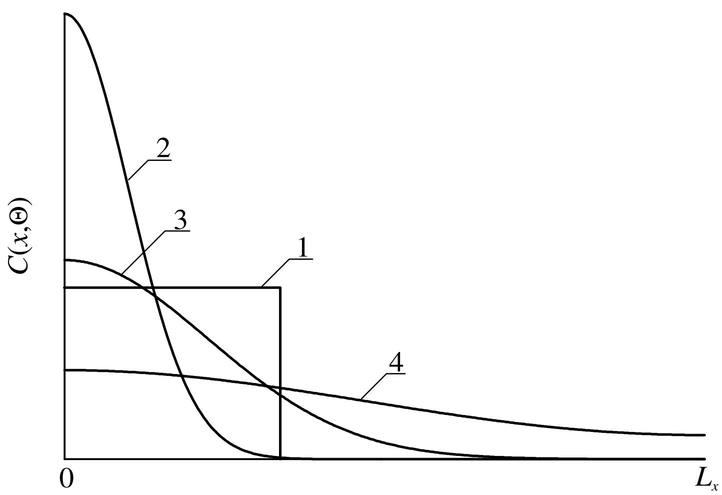

Fig. 4. Distributions of concentrations of infused dopant in the considered heterostructure. Curve 1 is the idealized distribution of dopant. Curves 2-4 are the real distributions of concentrations of dopant for different values of annealing time for increasing of annealing time with increasing of number of curve

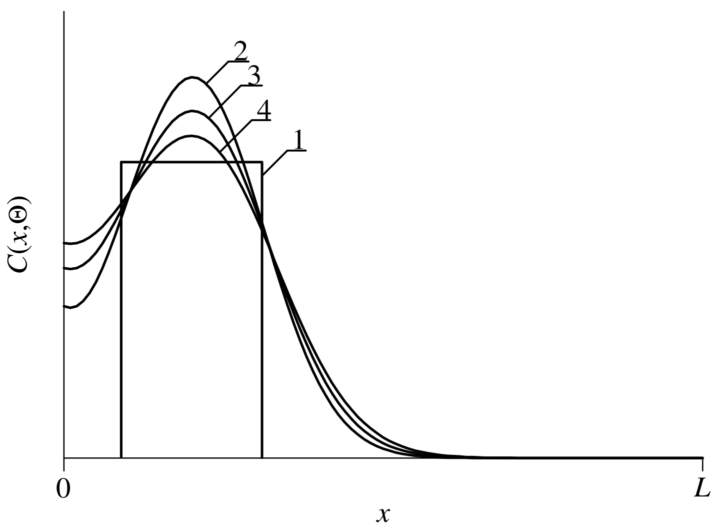

Fig. 5. Distributions of concentrations of implanted dopant in the considered heterostructure. Curve 1 is the idealized distribution of dopant. Curves 2-4 are the real distributions of concentrations of dopant for different values of annealing time for increasing of annealing time with increasing of number of curve

We analyzed optimal value of annealing time. The analysis shows, that optimal value of annealing time for ion type of doping is smaller, than optimal value of annealing time for diffusion type of doping. It is known, that ion doping of materials leads to radiation damage of doped materials. In this situation radiation defects should be annealed. The annealing leads to the above difference between optimal values of annealing time of dopant. The annealing of implanted dopant is necessary in the case, when the dopant did not achieved nearest interface between layers of heterostructure during annealing of radiation defects.

It should be noted, that using diffusion type of doping did not leads to radiation damage of materials. However radiation damage of materials during ion doping gives a possibility to decrease mismatch-induced stress in heterostructure [34].

4. CONCLUSIONS

In this paper we introduced an approach to decrease dimensions of a circuit XOR. The approach based on optimization of manufacturing field-effect heterotransistors, which includes into itself the considered circuit.

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