ON OPTIMIZATION OF DOPING OF A HETERO-STRUCTURE DURING MANUFACTURING OF *P-I-N*-DIODES

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ABSTRACT

We introduce an approach of manufacturing of a p-i-n-heterodiodes. The approach based on using a δ-doped heterostructure, doping by diffusion or ion implantation of several areas of the heterostructure. After the doping the dopant and/or radiation defects have been annealed. We introduce an approach to optimize annealing of the dopant and/or radiation defects. We determine several conditions to manufacture more compact p-i-n-heterodiodes.

KEYWORDS

p-i-n-heterodiodes; decreasing of dimensions of p-i-n-diodes; optimization of manufacturing; δ-doping; analytical approach for modelling

1. INTRODUCTION

Development of the solid state electronic devices leads to necessity of increasing of performance, reliability and integration rate of elements of integrated circuits (*p-n*- junctions, their systems et al) [1-7]. Increasing of integration rate of elements of integrated circuits leads to necessity to decrease their dimensions. One way to increase performance of the above elements is determination new materials with high charge carrier's motilities. The second one is elaboration new technological processes and optimization existing one [8-21]. Dimensions of elements of integrated circuits could be also decreased by using new technological processes and optimization existing one [8-17].

In the present paper we consider an approach to decrease dimensions of *p-i-n*-diodes. The approach based on using a heterostructure from Fig. 1. The heterostructure consist of a substrate and four epitaxial layers. A δ-layer has been grown between average epitaxial layers to manufacture required type of conductivity (*n* or *p*) in the doped area. Another epitaxial layers have been manufactured with sections (see Fig. 1). The sections have been manufactured by using another materials. We assumed, that the sections have been doped by diffusion or ion implantation to produce in this section required type of conductivity (*p* or *n*). The considered approach gives us possibility to manufacture more thin *p-i-n*-diodes. After doping sections dopant and/or radiation defects have been annealed. Annealing of dopant gives us possibility to infuse the dopant on required depth. Annealing of radiation defects gives us possibility to decrease their quantity. Framework this paper we analyzed dynamics of dopant and radiation defects during annealing.

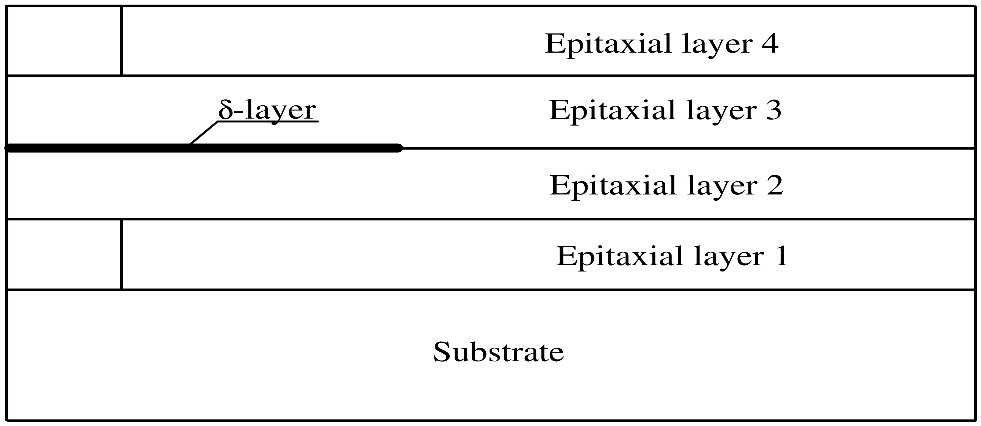

Fig. 1. A multilayer structure with a substrate and four epitaxial layers.
Heterostructure, which consist of a substrate, four epitaxial layers and sections framework the layers

2. METHOD OF SOLUTION

We determine distributions of concentrations of dopants in space and time to solve our aim. To determine the distributions we solved the second Fick's law [1,3,17]

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

Boundary and initial conditions for the equations are

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

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

The function $C(x,y,z,t)$ describes distribution of concentration of dopant in space and time; T is the temperature of annealing; D_C is the dopant diffusion coefficient. Dopant diffusion coefficient has different values in different materials. Value of dopant diffusion coefficient changing with heating and cooling of heterostructure (with account Arrhenius law). Dopant diffusion coefficient could be approximated by the following relation [22-24]

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

The function $D_L(x,y,z,T)$ describes variation of dopant diffusion coefficient in space (due inhomogeneity of heterostructure) and with variation of temperature (due to Arrhenius law); the function $P(x,y,z,T)$ describes the limit of solubility of dopant; parameter γ is integer in the following interval $\gamma\in[1,3]$ [22]; the function $V(x,y,z,t)$ describes variation of distribution of concentration of radiation vacancies in space and time; the parameter V^* describes the equilibrium distribution of concentration of vacancies. Dependence of dopant diffusion coefficient on concentration of dopant has been described in details in [22]. It should be noted, that using diffusion type of doping did not generation radiation defects. In this situation $\zeta_1=\zeta_2=0$. We determine distributions of concentrations of radiation defects in space and time by solving the following system of equations [23,24]

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

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

Boundary and initial conditions for these equations are

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

Here $\rho=I,V$; the function $I(x,y,z,t)$ describes distribution of concentration of radiation interstitials in space and time; $D_\rho(x,y,z,T)$ 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.

Distributions of concentrations of divacancies $\Phi_V(x,y,z,t)$ and dinterstitials $\Phi_I(x,y,z,t)$ in space and time have been determined by solving the following system of equations [23,24]

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

Boundary and initial conditions for these equations are

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

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

$$\frac{x\,y\,z}{L_x L_y L_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z} C(u,v,w,t)\,d\,w\,d\,v\,d\,u = \frac{y\,z}{L_y L_z}\int_{0}^{t}\int_{L_y}^{y}\int_{L_z}^{z}\left[1+\varsigma_1\frac{V(x,v,w,\tau)}{V^*}+\varsigma_2\frac{V^2(x,v,w,\tau)}{(V^*)^2}\right]\times$$

$$\times D_L(x,v,w,T)\left[1+\xi\frac{C^\gamma(x,v,w,\tau)}{P^\gamma(x,v,w,T)}\right]\frac{\partial\,C(x,v,w,\tau)}{\partial\,x}\,d\,\tau+\frac{x\,z}{L_x L_z}\int_{0}^{t}\int_{L_x}^{x}\int_{L_z}^{z} D_L(u,y,w,T)\times$$

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

$$+\frac{x\,y}{L_x L_y}\int_{0}^{t}\int_{L_x}^{x}\int_{L_y}^{y} D_L(u,v,z,T)\left[1+\varsigma_1\frac{V(u,v,z,\tau)}{V^*}+\varsigma_2\frac{V^2(u,v,z,\tau)}{(V^*)^2}\right]\left[1+\xi\frac{C^\gamma(u,v,z,\tau)}{P^\gamma(x,y,z,T)}\right]\times$$

$$\times\frac{\partial\,C(u,v,z,\tau)}{\partial\,z}d\,\tau+\frac{x\,y\,z}{L_x L_y L_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z} f(u,v,w)\,d\,w\,d\,v\,d\,u\,. \qquad (1a)$$

We determine solution of the above equation by using Bubnov-Galerkin approach [25]. Framework the approach we determine solution of the Eq.(1*a*) as the following series

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

where $e_{nC}(t)=\exp\left[-\pi^2 n^2 D_{0C} t\left(L_x^{-2}+L_y^{-2}+L_z^{-2}\right)\right]$, $c_n(\chi)=cos(\pi\, n\chi/L_\chi)$. 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 ξ=0) and averaged dopant diffusion coefficient D_0. Substitution of the series into Eq.(1*a*) leads to the following result

$$\frac{x\,y\,z}{\pi^2}\sum_{n=1}^{N}\frac{a_C}{n^3}s_n(x)\,s_n(y)\,s_n(z)\,e_{nC}(t)=-\frac{y\,z}{L_y L_z}\int_{0}^{t}\int_{L_y}^{y}\int_{L_z}^{z}\left\{1+\left[\sum_{n=1}^{N} a_{nC}\,c_n(x)\,c_n(v)\,c_n(w)\,e_{nC}(\tau)\right]^\gamma\times\right.$$

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

$$\times n\,c_n(w)\,e_{nC}(\tau)d\,\tau-\frac{x\,z}{L_x L_z}\int_{0}^{t}\int_{L_x}^{x}\int_{L_z}^{z}\left\{1+\left[\sum_{m=1}^{N} a_{mC}\,c_m(u)\,c_m(y)\,c_m(w)\,e_{mC}(\tau)\right]^\gamma\frac{\xi}{P^\gamma(u,y,w,T)}\right\}\times$$

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

$$\times a_{nC}-\frac{x\,y}{L_x L_y}\int_{0}^{t}\int_{L_x}^{x}\int_{L_y}^{y} D_L(u,v,z,T)\left\{1+\frac{\xi}{P^\gamma(u,v,z,T)}\left[\sum_{n=1}^{N} a_{nC}\,c_n(u)\,c_n(v)\,c_n(z)\,e_{nC}(\tau)\right]^\gamma\right\}\times$$

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

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

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

$$-\frac{L_x^2 L_y^2 L_z^2}{\pi^5}\sum_{n=1}^{N}\frac{a_{nC}}{n^6}e_{nC}(t)=-\frac{L_y L_z}{2\pi^2}\int_0^t\int_0^{L_x}\int_0^{L_y}\int_0^{L_z}D_L(x,y,z,T)\left\{1+\left[\sum_{n=1}^{N}a_{nC}\,c_n(x)\,c_n(y)\,c_n(z)\,e_{nC}(\tau)\right]^\gamma\times\right.$$
$$\left.\times\frac{\xi}{P^\gamma(x,y,z,T)}\right\}\left[1+\varsigma_1\frac{V(x,y,z,\tau)}{V^*}+\varsigma_2\frac{V^2(x,y,z,\tau)}{(V^*)^2}\right]\sum_{n=1}^{N}\frac{a_{nC}}{n}s_n(2x)\,c_n(y)\,c_n(z)\,e_{nC}(\tau)\times$$
$$\times\left\{y\,s_n(y)+\frac{L_y}{\pi n}[c_n(y)-1]\right\}\left\{z\,s_n(z)+\frac{L_z}{\pi n}[c_n(z)-1]\right\}d\,z\,d\,y\,d\,x\,d\,\tau-\int_0^t\int_0^{L_x}\int_0^{L_y}\int_0^{L_z}D_L(x,y,z,T)\times$$
$$\times D_L(x,y,z,T)\left\{1+\left[\sum_{n=1}^{N}a_{nC}\,c_n(x)\,c_n(y)\,c_n(z)\,e_{nC}(\tau)\right]^\gamma\frac{\xi}{P^\gamma(x,y,z,T)}\right\}\left[1+\varsigma_1\frac{V(x,y,z,\tau)}{V^*}+\right.$$
$$\left.+\varsigma_2\frac{V^2(x,y,z,\tau)}{(V^*)^2}\right]\left[1+\varsigma_1\frac{V(x,y,z,\tau)}{V^*}+\varsigma_2\frac{V^2(x,y,z,\tau)}{(V^*)^2}\right]\sum_{n=1}^{N}\left\{x\,s_n(x)+\frac{L_x}{\pi n}[c_n(x)-1]\right\}\frac{a_{nC}}{n}\times$$
$$\times\frac{L_x L_z}{2\pi^2}c_n(x)s_n(2y)\,c_n(z)\,e_{nC}(\tau)\left\{z\,s_n(z)+\frac{L_z}{\pi n}[c_n(z)-1]\right\}d\,z\,d\,y\,d\,x\,d\,\tau-\frac{L_x L_y}{2\pi^2}\times$$
$$\times\int_0^t\int_0^{L_x}\int_0^{L_y}\int_0^{L_z}\left\{1+\left[\sum_{n=1}^{N}a_{nC}\,c_n(x)\,c_n(y)\,c_n(z)\,e_{nC}(\tau)\right]^\gamma\frac{\xi}{P^\gamma(x,y,z,T)}\right\}\left[1+\varsigma_2\frac{V^2(x,y,z,\tau)}{(V^*)^2}+\right.$$
$$\left.+\varsigma_1\frac{V(x,y,z,\tau)}{V^*}\right]D_L(x,y,z,T)\sum_{n=1}^{N}\frac{a_{nC}}{n}c_n(x)\,c_n(y)\,s_n(z)\left\{x\,s_n(x)+\frac{L_x}{\pi n}[c_n(x)-1]\right\}\times$$
$$\times\left\{y\,s_n(y)+\frac{L_y}{\pi n}[c_n(y)-1]\right\}e_{nC}(\tau)d\,z\,d\,y\,d\,x\,d\,\tau+\sum_{n=1}^{N}\int_0^{L_x}\left\{x\,s_n(x)+\frac{L_x}{\pi n}[c_n(x)-1]\right\}\times$$
$$\times\int_0^{L_y}\left\{y\,s_n(y)+\frac{L_y}{\pi n}[c_n(y)-1]\right\}\int_0^{L_z}\left\{z\,s_n(z)+\frac{L_z}{\pi n}[c_n(z)-1]\right\}f(x,y,z)d\,z\,d\,y\,d\,x\ .$$

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

$$a_{nC}=\int_0^{L_x}\int_0^{L_y}\left\{y\,s_n(y)+\frac{L_y}{\pi n}[c_n(y)-1]\right\}\int_0^{L_z}\left\{z\,s_n(z)+\frac{L_y}{\pi n}[c_n(z)-1]\right\}f(x,y,z)d\,z\,d\,y\left\{x\,s_n(x)+\right.$$
$$\left.\times[c_n(x)-1]\frac{L_x}{\pi n}\right\}d\,x\left(\frac{n}{2}\left\{\int_0^t\int_0^{L_x}s_n(2x)\int_0^{L_y}c_n(y)\left\{y\,s_n(y)+\frac{L_y}{\pi n}[c_n(y)-1]\right\}\int_0^{L_z}D_L(x,y,z,T)\times\right.\right.$$
$$\times\left\{z\,s_n(z)+\frac{L_y}{\pi n}[c_n(z)-1]\right\}\left[1+\varsigma_1\frac{V(x,y,z,\tau)}{V^*}+\varsigma_2\frac{V^2(x,y,z,\tau)}{(V^*)^2}\right]\left[1+\frac{\xi}{P^\gamma(x,y,z,T)}\right]\times$$
$$\times c_n(z)d\,z\,d\,y\,d\,x\,e_{nC}(\tau)d\,\tau+\int_0^t e_{nC}(\tau)\int_0^{L_x}c_n(x)\left\{x\,s_n(x)+\frac{L_y}{\pi n}[c_n(x)-1]\right\}\int_0^{L_y}s_n(2y)\int_0^{L_z}c_n(z)\times$$
$$\times\left\{z\,s_n(z)+\frac{L_y}{\pi n}[c_n(z)-1]\right\}\left[1+\frac{\xi}{P^\gamma(x,y,z,T)}\right]\left[1+\varsigma_1\frac{V(x,y,z,\tau)}{V^*}+\varsigma_2\frac{V^2(x,y,z,\tau)}{(V^*)^2}\right]\times$$
$$\times D_L(x,y,z,T)\,d\,z\,d\,y\,d\,x\,d\,\tau+\int_0^t e_{nC}(\tau)\int_0^{L_x}c_n(x)\left\{x\,s_n(x)+\frac{L_x}{\pi n}[c_n(x)-1]\right\}\int_0^{L_y}c_n(y)\left\{s_n(y)\times\right.$$

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

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

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

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

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

$$\times c_n(x)\,s_n(2y)c_n(z)\frac{D_L(x,y,z,T)}{P(x,y,z,T)}\,d\,z\,d\,y\,d\,x\,d\,\tau+\frac{\xi L_xL_y}{2\pi^2n}\int_0^t e_{nC}(\tau)\int_0^{L_x}c_n(x)\int_0^{L_y}c_n(y)\int_0^{L_z}\frac{D_L(x,y,z,T)}{P(x,y,z,T)}\times$$

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

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

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

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

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

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

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

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. 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

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

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

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

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

$$+\frac{x\,y\,z}{L_x L_y L_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z} f_I(u,v,w)\,d\,w\,d\,v\,d\,u \qquad (4a)$$

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

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

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

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

$$+\frac{x\,y\,z}{L_x L_y L_z}\int_{L_x}^{x}\int_{L_y}^{y}\int_{L_z}^{z} f_V(u,v,w)\,d\,w\,d\,v\,d\,u\,.$$

We determine solutions of the Eqs.(4*a*) as the following series

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

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

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

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

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

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

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

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

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

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

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

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

We determine 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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

We determine solutions of the Eqs.(4*a*) as the following series

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

Coefficients $a_{n\Phi\rho}$ are not yet known. 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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$+L_y\Big\}\int\limits_0^{L_z}[1-c_n(2y)]D_{\Phi I}(x,y,z,T)\,d\,z\,d\,y\,d\,x\,e_{n\Phi I}(\tau)\,d\,\tau+\frac{1}{\pi^3}\sum_{n=1}^{N}\frac{a_{n\Phi I}}{n^3}\int\limits_0^t e_{n\Phi I}(\tau)\int\limits_0^{L_x}\Big\{\frac{L_x}{2\pi n}[c_n(x)-1]+$$

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

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

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

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

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

$$-\frac{L_x^2 L_y^2 L_z^2}{\pi^5}\sum_{n=1}^{N}\frac{a_{n\Phi V}}{n^6}e_{n\Phi V}(t)=-\frac{1}{2\pi L_x}\sum_{n=1}^{N}\int_0^t\int_0^{L_x}[1-c_n(2x)]\int_0^{L_y}\left\{L_y+y\,s_n(2y)+\frac{L_y}{2\pi n}[c_n(2y)-1]\right\}\times$$
$$\times\frac{a_{n\Phi V}}{n^2}\int_0^{L_z}D_{\Phi V}(x,y,z,T)\left\{z\,s_n(z)+\frac{L_z}{2\pi n}[c_n(z)-1]\right\}d\,z\,d\,y\,d\,x\,e_{n\Phi V}(\tau)\,d\,\tau-\frac{1}{2\pi}\sum_{n=1}^{N}\int_0^t\int_0^{L_x}\{x\,s_n(2x)+$$
$$+L_x+\frac{L_x}{2\pi n}[c_n(2x)-1]\Big\}\int_0^{L_y}[1-c_n(2y)]\int_0^{L_z}D_{\Phi V}(x,y,z,T)\left\{z\,s_n(z)+\frac{L_z}{2\pi n}[c_n(z)-1]\right\}d\,z\,d\,y\,d\,x\times$$
$$\times a_{n\Phi V}\frac{e_{n\Phi V}(\tau)}{n^2 L_y}d\,\tau-\frac{1}{2\pi L_x}\sum_{n=1}^{N}\frac{a_{n\Phi V}}{n^2}\int_0^t\int_0^{L_x}\left\{x\,s_n(x)+\frac{L_x}{2\pi n}[c_n(x)-1]\right\}\int_0^{L_y}\left\{y\,s_n(2y)+\frac{L_y}{2\pi n}[c_n(2y)-1]+\right.$$
$$\left.+L_y\right\}\int_0^{L_z}[1-c_n(2y)]D_{\Phi V}(x,y,z,T)d\,z\,d\,y\,d\,x\,e_{n\Phi V}(\tau)d\,\tau+\frac{1}{\pi^3}\sum_{n=1}^{N}\frac{a_{n\Phi V}}{n^3}\int_0^t e_{n\Phi V}(\tau)\int_0^{L_x}\left\{\frac{L_x}{2\pi n}[c_n(x)-1]+\right.$$
$$\left.+x\,s_n(x)\right\}\int_0^{L_y}\left\{y\,s_n(y)+\frac{L_y}{2\pi n}[c_n(y)-1]\right\}\int_0^{L_z}V^2(x,y,z,t)\,k_{V,V}(x,y,z,T)\left\{\frac{L_z}{2\pi n}[c_n(z)-1]+\right.$$
$$\left.+z\,s_n(z)\right\}d\,z\,d\,y\,d\,x-\frac{1}{\pi^3}\sum_{n=1}^{N}\frac{a_{n\Phi V}}{n^3}\int_0^t e_{n\Phi V}(\tau)\int_0^{L_x}\left\{x\,s_n(x)+\frac{L_x}{2\pi n}[c_n(x)-1]\right\}\int_0^{L_y}\left\{\frac{L_y}{2\pi n}[c_n(y)-1]+\right.$$
$$\left.+y\,s_n(y)\right\}\int_0^{L_z}\left\{z\,s_n(z)+\frac{L_z}{2\pi n}[c_n(z)-1]\right\}k_V(x,y,z,T)V(x,y,z,t)d\,z\,d\,y\,d\,x+\frac{1}{\pi^3}\sum_{n=1}^{N}\frac{a_{n\Phi V}}{n^3}\times$$
$$\times\int_0^t e_{n\Phi V}(\tau)\int_0^{L_x}\left\{x\,s_n(x)+\frac{L_x}{2\pi n}[c_n(x)-1]\right\}\int_0^{L_y}\left\{y\,s_n(y)+\frac{L_y}{2\pi n}[c_n(y)-1]\right\}\int_0^{L_z}\left\{\frac{L_z}{2\pi n}[c_n(z)-1]+\right.$$
$$\left.+z\,s_n(z)\right\}f_{\Phi V}(x,y,z)\,d\,z\,d\,y\,d\,x\,.$$

3. DISCUSSION

In this section we used relations from previous section for analysis of influence of parameters on distributions of concentrations of infused and implanted dopants. The typical distributions are presented on Figs. 2 and 3, respectively. The figures correspond to doping of one layer of two-layer structure with higher value of dopant diffusion coefficient in comparison with value of dopant diffusion coefficient in the second layer. The figures show, that using interface between layers of heterostructure leads to increasing of compactness of *p-i-n*-heterodiode. At the same time we homogeneity of distributions of concentrations of dopants in doped areas increases with decreasing of the homogeneity outside the enriched areas.

We note, that using the considered approach of manufacturing *p-i-n*-diodes leads to necessity to optimize annealing of dopant and/or radiation defects. Necessity of this optimization is following. Increasing of annealing time of dopant gives a possibility to obtain too homogenous distribution of concentration of dopant. If the annealing time is small, the dopant has not enough time to achieve interface between layers of heterostructure. In this situation one can not find any modification of distribution of concentration of dopant due to existing the interface. In this situation it is required optimization of annealing time. We optimize annealing time of dopant framework recently introduced criterion [26-35]. Dependences of optimal annealing time on parameters are presented on Figs. 4 and 5. Optimal annealing time of implanted dopant is smaller, than optimal annealing time of infused dopant. Reason of the difference is necessity of annealing of radiation defects. One can find spreading of distribution of concentration of dopant during annealing of radiation defects. In the ideal distribution of concentration of dopant achieves interface between layers of heterostructure during annealing of radiation defects. It is practicably to use additional annealing of dopant in the case, one the dopant has not enough time to achieve the interface. The Fig. 5 shows just dependences of optimal values of additional annealing time of dopant.

It is known, that using diffusion type of doping did not leads radiation damage of materials in comparison with ion type of doping. However ion doping of heterostructures attracted an interest for large difference of the lattice constant. In this case radiation damage leads to mismatch-induced stress [36].

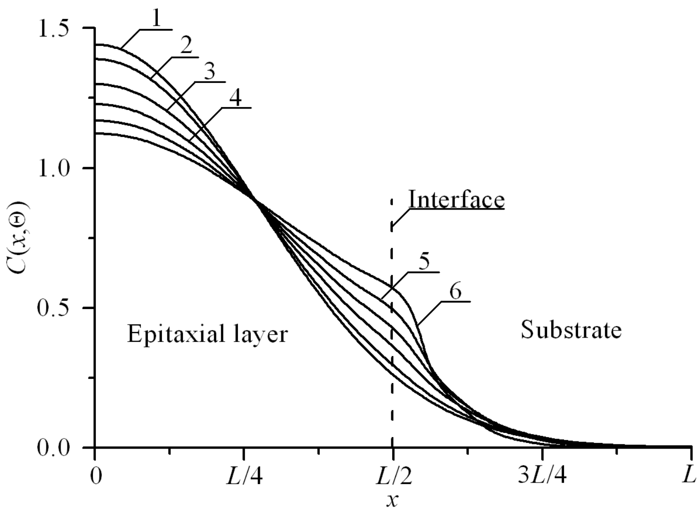

Fig.2. Dependences of concentration of infused dopant in heterostructure from Fig. 1 near one of interfaces. Value of dopant diffusion coefficient in the left layer is larger, than value of dopant diffusion coefficient in the right layer. Increasing of number of curve corresponds to increasing of difference between values of dopant diffusion coefficient in layers of heterostructure

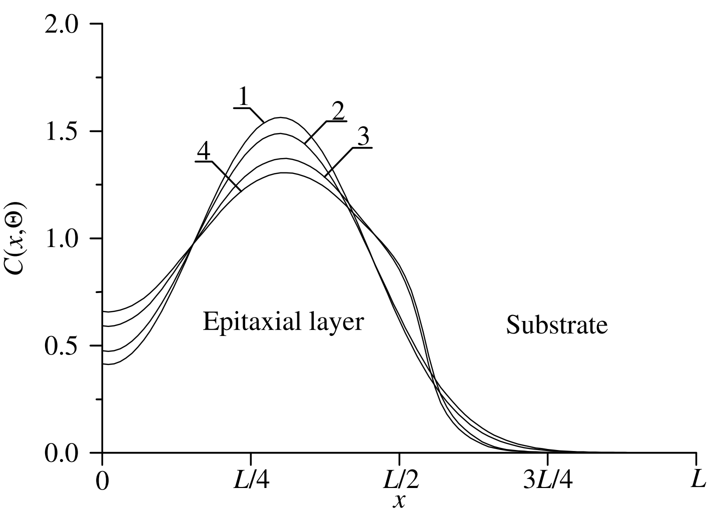

Fig.3. Dependence of concentration of implanted dopant on coordinate in heterostructure from Fig. 1 near one of interfaces. Curves 1 and 3 corresponds to annealing time $\Theta=0.0048(L_x^2+L_y^2+L_z^2)/D_0$. Curves 2 and 4 corresponds to annealing time $\Theta=0.0057(L_x^2+L_y^2+L_z^2)/D_0$. Curves 1 and 2 are distributions of concentration of implanted dopant in a homogenous sample. Curves 3 and 4 are distributions of concentration of implanted dopant in a heterostructure near one of interfaces. Value of dopant diffusion coefficient in the left layer is larger, than value of dopant diffusion coefficient in the right layer. Increasing of number of curve corresponds to increasing of difference between values of dopant diffusion coefficient in layers of heterostructure

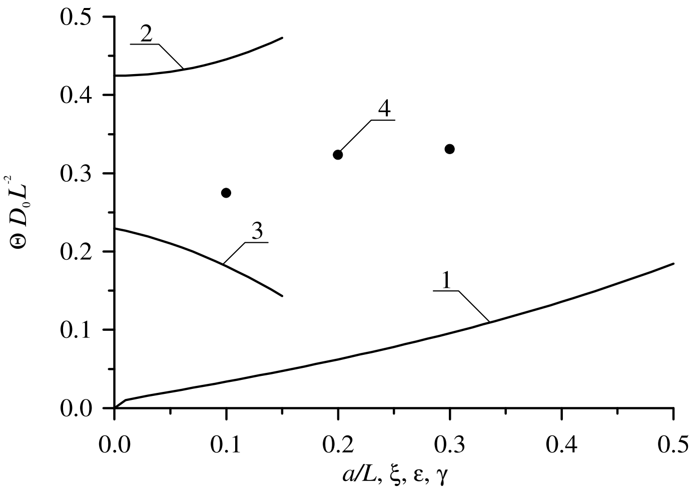

Fig.4. Optimal annealing time of infused dopant as a functions of several parameters. Curve 1 is the dependence of dimensionless optimal annealing time on the relation a/L and $\xi = \gamma = 0$ for equal to each other values of dopant diffusion coefficient in all parts of heterostructure. Curve 2 is the dependence of dimensionless optimal annealing time on value of parameter ε for a/L=1/2 and $\xi = \gamma = 0$. Curve 3 is the dependence of dimensionless optimal annealing time on value of parameter ξ for a/L=1/2 and $\varepsilon = \gamma = 0$. Curve 4 is the dependence of dimensionless optimal annealing time on value of parameter γ for a/L=1/2 and $\varepsilon = \xi = 0$

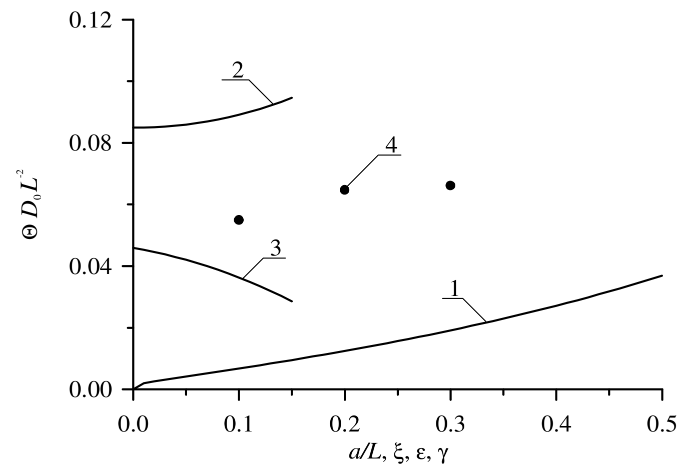

Fig.5. Optimal annealing time for ion doping of heterostructure as a function of several parameters. Curve 1 is the dependence of dimensionless optimal annealing time on the relation a/L and $\xi = \gamma = 0$ for equal to each other values of dopant diffusion coefficient in all parts of heterostructure. Curve 2 is the dependence of dimensionless optimal annealing time on value of parameter ε for a/L=1/2 and $\xi = \gamma = 0$. Curve 3 is the dependence of dimensionless optimal annealing time on value of parameter ξ for a/L=1/2 and $\varepsilon = \gamma = 0$. Curve 4 is the dependence of dimensionless optimal annealing time on value of parameter γ for a/L=1/2 and $\varepsilon = \xi = 0$

4. Conclusions

In this paper we introduce an approach to manufacture *p-i-n*-heterodiodes. The approach based on using a δ-doped heterostructure, doping by diffusion or ion implantation of several areas of the heterostructure. After the doping the dopant and/or radiation defects have been annealed.At the same time we consider an analytical approach to model technological processes. Framework the approach gives a possibility to manage without stitching decisions on the interfaces between layers heterostructures.

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