ON PROGNOSIS OF VARIATION OF DISTRIBUTION OF DOPANT IN A MULTILAYER STRUCTURE WITH CHANGING OVERGROWTH REGIME

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ABSTRACT

In this paper we analyzed redistribution of dopant in a multilayer structure during overgrowing of doped area. We analyzed the effect of changing of regimes of overgrowing of the doped area on the redistribution of dopant (changing of speed of overgrowth, changing of temperature of overgrowth). We introduce an analytical approach for analysis of redistribution of dopant. The approach gives a possibility to simultaneously taking into account the changing of parameters of the considered process (diffusion coefficient of dopant and radiation defects, limit of solubility of dopant, parameters of interaction between radiation defects) in space (due to presents of several layers in the considered multilayer structure) and time (due to variation of temperature of overgrowth in time), as well as nonlinearity of the mass transport (due to interaction between radiation defects and dopant).

KEYWORDS

multilayer structure, ion doping, overgrowth, analytical approach for modeling

1. INTRODUCTION

Currently, one of the intensively solved issues of solid-state electronics is increasing of performance of electronic devices: diodes, field-effect and bipolar transistors, ... and increasing of their density in the framework of integrated circuits. Refs. [1-6] describe manufacturing of integrated circuits. To increase the performance of the considered devices, it is possible to use materials with larger values of charge carrier mobility (Refs. [7-10] describe properties of materials) and new technological processes or modification of existing processes (one of the ways to decrease size of elements of integrated circuit is their manufacturing in the framework of thin-film multilayer structures [3-5,11]). In this case, inhomogeneity of multilayer structures was used, but it is necessary to optimize doping of electronic materials (Refs. [12] describe the considered optimization of technological process), as well as the development of epitaxial technology in order to improve properties of these materials (including the analysis of mismatch-induced stresses). Refs. [13-15] describe epitaxial technology. An alternative way to decrease dimensions of elements of integrated circuit is using of laser and microwave types of annealing. Laser and microwave types of annealing were described in Refs. [16-18]. In this paper we consider a two-layer structure, which consist of a substrate and an epitaxial layer (see Figure 1). A dopant was implanted into the epitaxial layer to produce the required type of conductivity in the layer. After that we consider high-temperature overgrowth of the epitaxial layer. Such an overgrowth would make it possible not to anneal radiation defects generated during implantation of dopant. The main aim of this pa-

per is analysis of redistribution of dopant diring overgrowth. The accompanying aim of this paper is to formation of an analytical approach for analysis of mass transfer with account changes in its parameters in space and time, as well as its nonlinearity.



Fig. 1. Considered multilayer structure with substrate, doped epitaxial layer and overlayer

2. METHOD OF SOLUTION

To solve our aims we will calculate the distribution of dopant in space and time in the considerate multilayer structure and analyze it. The distribution of concentration of dopant C(x,t) in space and time was calculated by solving Fick's second law (see the law in Refs. [1,15-17])

$$\frac{\partial C(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[D \frac{\partial C(x,t)}{\partial x} \right],\tag{1}$$

with boundary and initial conditions

$$\frac{\partial C(x,t)}{\partial x}\Big|_{x=-vt} = 0, \ \frac{\partial C(x,t)}{\partial x}\Big|_{x=L} = 0, \ C(x,0)=f(x).$$
(2)

where D(x) is the diffusion coefficient of dopant in the considered multilayer structure; v is the speed of overgrowth of epitaxial layer. Spatial distribution of the dopant diffusion coefficient depends on properties of layers of the considered multilayer structure; changing of temperature of overgrowth; redistribution of radiation defects, which were generated during ion implantation of dopant

$$D_{c} = D_{L}(x,T) \left[1 + \xi \frac{C^{\gamma}(x,t)}{P^{\gamma}(x,T)} \right] \left[1 + \zeta_{1} \frac{V(x,t)}{V^{*}} + \zeta_{2} \frac{V^{2}(x,t)}{(V^{*})^{2}} \right],$$
(3)

where $D_L(x,T)$ is the spatial (due to inhomogeneity of multilayer structure) and temperature (with account Arrhenius law) dependences of diffusion coefficient; *T* is the temperature of overgrowth; P(x,T) is the limit of solubility of dopant; parameter γ describes average quantity of charged defects interacted with atom of dopant and could be integer in the following interval $\gamma \in [1,3]$ (the dependence was described in details in [18]); function V(x,t) is the distribution of concentration of radiation vacancies space and time with equilibrium distribution V^* . Concentrational dependence of diffusion coefficient of dopant was considered in details in [18]. In this situation the

boundary problem (1)-(3) gives a possibility to analyze the considered process in more common case in comparison with models in Refs. [1,16,17,19]. We determine distribution of concentration of radiation defects in space and time by solving of the following system of equations (the considered equations were considered in details in Refs. [1,16,17,19])

$$\begin{cases}
\frac{\partial I(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[D_{I}(x,T) \frac{\partial I(x,t)}{\partial x} \right] - k_{I,I}(x,T) I^{2}(x,t) - k_{I,V}(x,T) I(x,t) V(x,t) \\
\frac{\partial V(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[D_{V}(x,T) \frac{\partial V(x,t)}{\partial x} \right] - k_{V,V}(x,T) I^{2}(x,t) - k_{I,V}(x,T) I(x,t) V(x,t)
\end{cases}$$
(4)

with boundary and initial conditions

$$\frac{\partial I(x,t)}{\partial x}\Big|_{x=-vt} = 0, \ \frac{\partial I(x,t)}{\partial x}\Big|_{x=L} = 0, \ \frac{\partial V(x,t)}{\partial x}\Big|_{x=-vt} = 0, \ \frac{\partial V(x,t)}{\partial x}\Big|_{x=L} = 0,$$

$$I(x,0) = f_I(x), \ V(x,0) = f_V(x).$$
(5)

Function I(x,t) describes distribution of concentration of radiation interstitials in space and time with equilibrium distribution I^* ; $D_I(x,T)$, $D_V(x,T)$ are the diffusion coefficients of interstitials and vacancies; terms $V^2(x,t)$ and $I^2(x,t)$ correspond to generation divacancies and diinterstitials (see [17] and appropriate references in this book); function $k_{I,V}(x,T)$ is the parameter of recombination of point radiation defects; functions $k_{I,I}(x,T)$ and $k_{V,V}(x,T)$ are the parameters of generation of simplest complexes of point radiation defects. In this situation the boundary problem (4)-(5) gives a possibility to analyze the considered process in more common case in comparison with models in Refs. [1,16,17,19]. Distributions of concentration of divacancies $\Phi_V(x,t)$ and analogous complexes of interstitials $\Phi_I(x,t)$ in space and time were determined as solution of the following system of equations (the considered equations were considered in details in Refs. [16,17,19])

$$\begin{cases} \frac{\partial \Phi_{I}(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[D_{\Phi_{I}}(x,T) \frac{\partial \Phi_{I}(x,t)}{\partial x} \right] + k_{I,I}(x,T) I^{2}(x,t) + k_{I}(x,T) I(x,t) \\ \frac{\partial \Phi_{V}(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[D_{\Phi_{V}}(x,T) \frac{\partial \Phi_{V}(x,t)}{\partial x} \right] + k_{V,V}(x,T) V^{2}(x,t) + k_{V}(x,T) V(x,t) \end{cases}$$
(6)

with boundary and initial conditions

$$\frac{\partial \Phi_{I}(x,t)}{\partial x}\Big|_{x=-vt} = 0, \ \frac{\partial \Phi_{I}(x,t)}{\partial x}\Big|_{x=L} = 0, \ \frac{\partial \Phi_{V}(x,t)}{\partial x}\Big|_{x=-vt} = 0, \ \frac{\partial \Phi_{V}(x,t)}{\partial x}\Big|_{x=L} = 0, \quad (7)$$

$$\Phi_{I}(x,0) = f_{\Phi I}(x), \ \Phi_{V}(x,0) = f_{\Phi V}(x).$$

Here $D_{\phi l}(x,T)$ and $D_{\phi V}(x,T)$ are the diffusion coefficients of complexes of point radiation defects; $k_l(x,T)$ and $k_V(x,T)$ are the parameters of decay of the considered complexes. In this situation the boundary problem (6)-(7) gives a possibility to analyze the considered process in more common case in comparison with models in Refs. [16,17,19].

To analyze redistribution of dopant in different regimes of overgrowth of epitaxial layer one shall to calculate solution of Eq. (1). It is attracted an interest replacement of variations x and t and dif-

fusion coefficients by dimentionless variables χ and \mathscr{G} and normalized diffusion coefficients: $x \rightarrow \chi = (x+vt)/L$, $t \rightarrow \mathscr{G} = tD_0/L^2$ and $\Delta c = D_L(x,T)/D_0$, where D_0 is the average value of dopant diffusion coefficient. Using the considered replacement leads to transformation of Eq. (1) to the following form

$$\frac{\partial C(\chi, \theta)}{\partial \theta} = \frac{\partial}{\partial \chi} \left[\Delta_C(\chi, T) \frac{\partial C(\chi, \theta)}{\partial \chi} \right] + \frac{\nu L}{D_0} \frac{\partial C(\chi, \theta)}{\partial \theta}.$$
(1*a*)

Boundary and initial conditions dimentionless variables takes the form

$$\frac{\partial C(\chi, \theta)}{\partial \chi}\Big|_{\chi=0} = 0, \ \frac{\partial C(\chi, \theta)}{\partial \chi}\Big|_{\chi=1-\nu t/L} = 0, \ C(\chi, 0) = f(\chi).$$
(2a)

One can neglect by term v t /L in comparison with 1 near boundary x=L (i.e. $\chi =1-v t /L$) of the considered multilayer structure. The approximation gives a possibility to re-write the second boundary condition in the following form $\partial C (\chi, \theta)/\partial \chi |_{\chi=1} \approx 0$ and to analyzed redistribution of dopant in the considered moving area with the single length. The considered replacement of variable leads to the following transformation of Eqs. (4) and (6) and appropriate conditions

$$\left| \frac{\partial I\left(\chi, \vartheta\right)}{\partial \vartheta} = \frac{\partial}{\partial \chi} \left[\Delta_{I}\left(\chi, T\right) \frac{\partial I\left(\chi, \vartheta\right)}{\partial \chi} \right] + \frac{vL}{D_{0}} \frac{\partial I\left(\chi, \vartheta\right)}{\partial \vartheta} - \frac{-k_{I,I}\left(\chi, T\right)I^{2}\left(\chi, \vartheta\right) - k_{I,V}\left(\chi, T\right)I\left(\chi, \vartheta\right)V\left(\chi, \vartheta\right)}{\partial \vartheta} - \frac{-k_{I,I}\left(\chi, T\right)V^{2}\left(\chi, \vartheta\right) - k_{I,V}\left(\chi, T\right)I\left(\chi, \vartheta\right)V\left(\chi, \vartheta\right)}{\partial \vartheta} - \frac{-k_{V,V}\left(\chi, T\right)V^{2}\left(\chi, \vartheta\right) - k_{I,V}\left(\chi, T\right)I\left(\chi, \vartheta\right)V\left(\chi, \vartheta\right)}{\partial \chi} \right|_{\chi=0} = 0, \quad \frac{\partial I\left(\chi, \vartheta\right)}{\partial \chi} \right|_{\chi=1} = 0, \quad \frac{\partial V\left(\chi, \vartheta\right)}{\partial \chi} \right|_{\chi=0} = 0, \quad \frac{\partial I\left(\chi, \vartheta\right)}{\partial \chi} \right|_{\chi=1} = 0, \quad \frac{\partial V\left(\chi, \vartheta\right)}{\partial \chi} \right|_{\chi=0} = 0, \quad \frac{\partial V\left(\chi, \vartheta\right)}{\partial \chi} \right|_{\chi=1} = 0, \quad (5a)$$

$$\frac{\partial \Phi_{I}\left(\chi, \vartheta\right)}{\partial \vartheta} = \frac{\partial}{\partial \chi} \left[\Delta_{\Phi_{V}}\left(\chi, T\right) \frac{\partial \Phi_{I}\left(\chi, \vartheta\right)}{\partial \chi} \right] + \frac{vL}{D_{0}} \frac{\partial \Phi_{I}\left(\chi, \vartheta\right)}{\partial \vartheta} + \frac{k_{I,I}\left(\chi, T\right)I^{2}\left(\chi, \vartheta\right) + k_{I}\left(\chi, T\right)I\left(\chi, \vartheta\right)}{\partial \vartheta} + \frac{k_{V,V}\left(\chi, T\right)V^{2}\left(\chi, \vartheta\right) + k_{V}\left(\chi, T\right)I\left(\chi, \vartheta\right)}{\partial \vartheta} + \frac{\partial \Phi_{V}\left(\chi, \vartheta\right)}{\partial \chi} \right|_{\chi=0} = 0, \quad \frac{\partial \Phi_{V}\left(\chi, \vartheta\right)}{\partial \chi} \right|_{\chi=0} = 0, \quad (7a)$$

$$\frac{\partial \Phi_{I}\left(\chi, \vartheta\right)}{\partial \chi} \right|_{\chi=0} = 0, \quad \frac{\partial \Phi_{I}\left(\chi, \vartheta\right)}{\partial \chi} \right|_{\chi=1} = 0, \quad \frac{\partial \Phi_{V}\left(\chi, \vartheta\right)}{\partial \chi} \right|_{\chi=0} = 0, \quad \frac{\partial \Phi_{V}\left(\chi, \vartheta\right)}{\partial \chi} \right|_{\chi=1} = 0, \quad (7a)$$

To estimate distribution of dopant in space and time analytical approaches of solution attracts priority interests in comparison with numerical one due to higher visibility. We used the method of averaging of function corrections (the approach was considered in details in Refs. [15,20]) to solve Eqs. (1*a*), (4*a*), (6*a*). In the framework of the approach we replace the required concentrations in right sides of the considered equations on their not yet known average values $\alpha_{1\rho}$. In this

case we obtain equations to calculate the first-order approximations for considered functions. They could be written in the following form

$$\frac{\partial C_1(\chi, \vartheta)}{\partial \vartheta} = 0 \tag{1b}$$

$$\begin{cases} \frac{\partial I_{I}(\chi, \vartheta)}{\partial \vartheta} = -\alpha_{II}^{2} k_{I,I}(\chi, T) - \alpha_{II} \alpha_{IV} k_{I,V}(\chi, T) \\ \frac{\partial V_{I}(\chi, \vartheta)}{\partial \vartheta} = -\alpha_{IV}^{2} k_{V,V}(\chi, T) - \alpha_{II} \alpha_{IV} k_{I,V}(\chi, T) \end{cases}$$

$$\begin{cases} \frac{\partial \Phi_{II}(\chi, \vartheta)}{\partial \vartheta} = k_{I,I}(\chi, T) I^{2}(\chi, \vartheta) + k_{I}(\chi, T) I(\chi, \vartheta) \\ \frac{\partial \Phi_{IV}(\chi, \vartheta)}{\partial \vartheta} = k_{V,V}(\chi, T) V^{2}(\chi, \vartheta) + k_{V}(\chi, T) I(\chi, \vartheta) \end{cases}$$
(6b)

Integration of left and right sides of the above equations on normalized time \mathcal{G} gives a possibility to obtain the first-order approximations of the considered approximations in the final form

$$C_{1}(\chi, \mathcal{G}) = f(\chi) \tag{1c}$$

$$\begin{cases} I_{I}(\chi, \vartheta) = f_{I}(\chi) - \alpha_{II}^{2} \int_{0}^{\vartheta} k_{I,I}(\chi, T) d\tau - \alpha_{II} \alpha_{IV} \int_{0}^{\vartheta} k_{I,V}(\chi, T) d\tau \\ V_{I}(\chi, \vartheta) = f_{V}(\chi) - \alpha_{IV}^{2} \int_{0}^{\vartheta} k_{V,V}(\chi, T) d\tau - \alpha_{II} \alpha_{IV} \int_{0}^{\vartheta} k_{I,V}(\chi, T) d\tau \end{cases}$$

$$(4c)$$

$$\begin{cases} \Phi_{1I}(\chi, \mathcal{G}) = \int_{0}^{\mathcal{G}} k_{I,I}(\chi, T) I^{2}(\chi, \tau) d\tau + \int_{0}^{\mathcal{G}} k_{I}(\chi, T) I(\chi, \tau) d\tau + f_{\Phi_{I}}(\chi) \\ \Phi_{1V}(\chi, \mathcal{G}) = \int_{0}^{\mathcal{G}} k_{V,V}(\chi, T) V^{2}(\chi, \tau) d\tau + \int_{0}^{\mathcal{G}} k_{V}(\chi, T) V(\chi, \tau) d\tau + f_{\Phi_{V}}(\chi) \end{cases}$$
(6c)

Average values of the first-order approximations of concentrations of dopant and radiation defects could be determined by using the following standard relation (the relation was considered in details in Refs. [15,20])

$$\alpha_{1\rho} = \frac{1}{\Theta} \int_{00}^{\Theta_1} \rho_1(\chi, \vartheta) d\chi d\vartheta, \qquad (8)$$

where Θ is the continuance of monitoring of the technological process. Substitution of functions (1*c*), (4*c*) and (6*c*) into relation (8) gives a possibility to obtain relations for not yet known average values of the considered concentrations on the following form

$$\alpha_{1C} = \int_{0}^{1} f(\chi) d\chi, \ \alpha_{1I} = \frac{\sqrt{(1+b\alpha_{1V})^{2} - 4a_{I}\int_{0}^{1} f_{I}(\chi) d\chi} - (1+b\alpha_{1V})}{2a_{I}},$$
$$\alpha_{1V} = \sqrt[3]{\sqrt{\frac{p^{3}}{27} + \frac{q^{2}}{4}} - \frac{q}{2}} - \sqrt[3]{\sqrt{\frac{p^{3}}{27} + \frac{q^{2}}{4}} + \frac{q}{2}} + \frac{b^{3} - (b - 2a_{V}a_{I})(b - 2a_{I})}{2[b^{2} + (2a_{I}a_{V} - b^{2})^{2}]},$$

$$\alpha_{1\Phi_{I}} = \int_{0}^{\Theta} \left(1 - \frac{9}{\Theta}\right)_{0}^{1} k_{I,I}(\chi, T) I^{2}(\chi, 9) d\chi d\theta + \int_{0}^{1} f_{\Phi_{I}}(\chi) d\chi + \int_{0}^{\Theta} \left(1 - \frac{9}{\Theta}\right)_{0}^{1} k_{I}(\chi, T) I(\chi, 9) d\chi d\theta$$
(9)
$$\alpha_{1\Phi_{V}} = \int_{0}^{\Theta} \left(1 - \frac{9}{\Theta}\right)_{0}^{1} k_{V,V}(\chi, T) V^{2}(\chi, 9) d\chi d\theta + \int_{0}^{1} f_{\Phi_{V}}(\chi) d\chi + \int_{0}^{\Theta} \left(1 - \frac{9}{\Theta}\right)_{0}^{1} k_{V}(\chi, T) V(\chi, 9) d\chi d\theta$$
(9)

where
$$a_{\rho} = \int_{0}^{\Theta} \left(1 - \frac{9}{\Theta}\right)_{0}^{1} k_{\rho,\rho}(\chi,T) d\chi d\theta$$
, $b = \int_{0}^{\Theta} \left(1 - \frac{9}{\Theta}\right)_{0}^{1} k_{I,V}(\chi,T) d\chi d\theta$, $p = \left(1 - \frac{b}{2a_{I}}\right)_{0}^{1} f_{V}(\chi) d\chi \times \left(\frac{b^{2}}{4a_{I}^{2}} + \left(a_{V} - \frac{b^{2}}{2a_{I}}\right)^{2}\right)^{-1} - \frac{1}{3} \left\{ \left[\frac{b^{2}}{4a_{I}^{2}} - \frac{b^{2}}{a_{I}}\right]_{0}^{1} f_{I}(\chi) d\chi \right] - \left(\frac{b}{2a_{I}} - 1\right)^{2} + 2\left(a_{V} + \frac{b^{2}}{2a_{I}}\right)_{0}^{1} f_{V}(\chi) d\chi \right\}^{2} \left[\frac{b^{2}}{4a_{I}^{2}} + \left(a_{V} - \frac{b^{2}}{2a_{I}}\right)^{2} \right]^{-2}, q = \frac{2}{27} \left\{ \left[\frac{b^{2}}{4a_{I}^{2}} - \frac{b^{2}}{a_{I}}\right]_{0}^{1} f_{I}(\chi) d\chi \right] - \left(\frac{b}{2a_{I}} - 1\right)^{2} + 2\left(a_{V} + \frac{b^{2}}{2a_{I}}\right)_{0}^{1} f_{V}(\chi) d\chi \right\}^{3} \left[\frac{b^{2}}{4a_{I}^{2}} + \left(a_{V} - \frac{b^{2}}{2a_{I}}\right)^{2} \right]^{-2}, q = \frac{2}{27} \left\{ \left[\frac{b^{2}}{4a_{I}^{2}} - \frac{b^{2}}{a_{I}}\right]_{0}^{1} f_{I}(\chi) d\chi \right] - \left(\frac{b}{2a_{I}} - 1\right)^{2} - 2\left(\frac{b}{2a_{I}} - a_{V}\right)_{0}^{1} f_{V}(\chi) d\chi \right\}^{3} \left[\frac{b^{2}}{4a_{I}^{2}} + \left(a_{V} - \frac{b^{2}}{2a_{I}}\right)^{2} \right]^{-3} - \left[\int_{0}^{1} f_{V}(\chi) d\chi \right]^{2} \left[\frac{b^{2}}{4a_{I}^{2}} + \left(a_{V} - \frac{b^{2}}{2a_{I}}\right)^{2} \right]^{-1} - \frac{2}{3} \left[\frac{b^{2}}{4a_{I}^{2}} + \left(a_{V} - \frac{b^{2}}{2a_{I}}\right)^{2} \right]^{-3} - \left[\int_{0}^{1} f_{V}(\chi) d\chi \right]^{2} \left[\frac{b^{2}}{4a_{I}^{2}} + \left(a_{V} - \frac{b^{2}}{2a_{I}}\right)^{2} \right]^{-1} - \frac{2}{3} \left[\frac{b^{2}}{4a_{I}^{2}} + \left(a_{V} - \frac{b^{2}}{2a_{I}}\right)^{2} \right]^{-1} \left\{ 2\left(a_{V} - \frac{b}{2a_{I}}\right)^{2} \right]^{-1} \left\{ 2\left(a_{V} - \frac{b}{2a_{I}}\right)^{2} \right]^{-1} \left\{ 2\left(a_{V} - \frac{b}{2a_{I}}\right)^{2} \right]^{-1} \left\{ 2\left(a_{V} - \frac{b^{2}}{2a_{I}}\right)^{2} \right]^{-1} \left\{ \frac{b^{2}}{2a_{I}} - 1\right)^{2} + \left[\frac{1}{4a_{I}} - \frac{1}{0} f_{I}(\chi) d\chi \right] \right\} - \left(\frac{b^{2}}{2a_{I}}\right)^{2} - 2\left(\frac{b^{2}}{2a_{I}} - 1\right)^{2} \left\{ \frac{b^{2}}{2a_{I}^{2}} + \left(a_{V} - \frac{b^{2}}{2a_{I}^{2}}\right)^{2} \right]^{-1} \left\{ \frac{b^{2}}{2a_{I}^{2}} - \frac{b^{2}}{2a_{I}^{2}} \right\} - \left(\frac{b^{2}}{2a_{I}^{2}} - \frac{b^{2}}{2a_{I}^{2}}\right)^{2} - 2\left(\frac{b^{2}}{2a_{I}^{2}} - \frac{b^{2}}{2a_{I}^{2}}\right)^{2} \left[\frac{b^{2}}{2a_{I}^{2}} + \left(a_{V} - \frac{b^{2}}{2a_{I}^{2}}\right)^{2} \right]^{-1} \left\{ \frac{b^{2}}{2a_{I}^{2}} - \frac{b^{2}}{2a_{I}^{2}} + \left(a_{V} - \frac{b^{2}}{2a_{I}^{2}}\right)^{2} \right]^{-1} \left\{ \frac{b^{2}}{2a_{I}^{2}} + \left(a_{V} - \frac{b^{2}}{2a_{I}$

To calculate the second-order approximations of concentrations of dopant and radiation defects one shall to replace the considered functions in the right sides of Eqs. (1a), (4a), (6a) on the sum of the not yet known average values of the considered approximations and approximations with the previous order. Analogous way could be used to calculate approximations with higher orders (larger, than 2). Equations to calculate the considered second-order approximations could be written as

$$\frac{\partial C_{2}(\chi, \vartheta)}{\partial \vartheta} = \frac{\partial}{\partial \chi} \left\{ \Delta_{c}(\chi, T) \left\{ 1 + \xi \frac{[\alpha_{2c} + C_{1}(\chi, \vartheta)]^{\gamma}}{P^{\gamma}(\chi, T)} \right\} \left[1 + \zeta_{1} \frac{V(\chi, \vartheta)}{V^{*}} + \zeta_{2} \frac{V^{2}(\chi, \vartheta)}{(V^{*})^{2}} \right] \times \frac{\partial C_{1}(\chi, \vartheta)}{\partial \chi} \right\} + \frac{vL}{D_{0}} \frac{\partial C_{1}(\chi, \vartheta)}{\partial \vartheta}$$

$$(1d)$$

$$\begin{cases} \frac{\partial I_{2}(\chi, \vartheta)}{\partial \vartheta} = \frac{\partial}{\partial \chi} \left[\Delta_{I}(\chi, T) \frac{\partial I_{1}(\chi, \vartheta)}{\partial \chi} \right] + \frac{\nabla L}{D_{0}} \frac{\partial I_{1}(\chi, \vartheta)}{\partial \vartheta} - \\ -k_{I,I}(\chi, T) [\alpha_{2I} + I_{1}(\chi, \vartheta)]^{2} - k_{I,V}(\chi, T) [\alpha_{2I} + I_{1}(\chi, \vartheta)] [\alpha_{2V} + V_{1}(\chi, \vartheta)] \\ \frac{\partial V_{2}(\chi, \vartheta)}{\partial \vartheta} = \frac{\partial}{\partial \chi} \left[\Delta_{V}(\chi, T) \frac{\partial V_{1}(\chi, \vartheta)}{\partial \chi} \right] + \frac{\nabla L}{D_{0}} \frac{\partial V_{1}(\chi, \vartheta)}{\partial \vartheta} - \\ -k_{V,V}(\chi, T) [\alpha_{2V} + V_{1}(\chi, \vartheta)]^{2} - k_{I,V}(\chi, T) [\alpha_{2I} + I_{1}(\chi, \vartheta)] [\alpha_{2V} + V_{1}(\chi, \vartheta)] \end{cases}$$
(4d)

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$$\begin{cases}
\frac{\partial \Phi_{2I}(\chi, \theta)}{\partial \theta} = \frac{\partial}{\partial \chi} \left[\Delta_{\Phi_{I}}(\chi, T) \frac{\partial \Phi_{II}(\chi, \theta)}{\partial \chi} \right] + \frac{vL}{D_{0}} \frac{\partial \Phi_{II}(\chi, \theta)}{\partial \theta} + \\
+ k_{I,I}(\chi, T)I^{2}(\chi, \theta) + k_{I}(\chi, T)I(\chi, \theta) \\
\frac{\partial \Phi_{2V}(\chi, \theta)}{\partial \theta} = \frac{\partial}{\partial \chi} \left[\Delta_{\Phi_{V}}(\chi, T) \frac{\partial \Phi_{IV}(\chi, \theta)}{\partial \chi} \right] + \frac{vL}{D_{0}} \frac{\partial \Phi_{IV}(\chi, \theta)}{\partial \theta} + \\
+ k_{V,V}(\chi, T)V^{2}(\chi, \theta) + k_{V}(\chi, T)I(\chi, \theta)
\end{cases}$$
(6d)

Integration of the left and right sides of the obtained equations on time gives a possibility to obtained the second-order approximations of the considered approximations in the following form

$$C_{2}(\chi, \vartheta) = \frac{\partial}{\partial \chi} \int_{0}^{\vartheta} \Delta_{c}(\chi, T) \left\{ 1 + \xi \frac{[\alpha_{2c} + C_{1}(\chi, \tau)]^{r}}{P^{r}(\chi, T)} \right\} \left[1 + \varsigma_{1} \frac{V(\chi, \tau)}{V^{*}} + \varsigma_{2} \frac{V^{2}(\chi, \tau)}{(v^{*})^{2}} \right] \frac{\partial C_{1}(\chi, \tau)}{\partial \chi} d\tau + \\ + \frac{vL}{D_{0}} C_{1}(\chi, \vartheta) + f_{c}(\chi)$$

$$(1e)$$

$$\begin{cases} I_{2}(\chi, \vartheta) = \frac{\partial}{\partial \chi} \int_{0}^{\vartheta} \Delta_{I}(\chi, T) \frac{\partial I_{1}(\chi, \tau)}{\partial \chi} d\tau - \int_{0}^{\vartheta} k_{I,I}(\chi, T) [\alpha_{2I} + I_{1}(\chi, \tau)]^{2} d\tau + \\ + f_{I}(\chi) + \frac{vL}{D_{0}} I_{1}(\chi, \vartheta) - \int_{0}^{\vartheta} k_{I,V}(\chi, T) [\alpha_{2I} + I_{1}(\chi, \tau)] [\alpha_{2V} + V_{1}(\chi, \tau)] d\tau \\ V_{2}(\chi, \vartheta) = \frac{\partial}{\partial \chi} \int_{0}^{\vartheta} \Delta_{V}(\chi, T) \frac{\partial V_{1}(\chi, \tau)}{\partial \chi} d\tau - \int_{0}^{\vartheta} k_{V,V}(\chi, T) [\alpha_{2V} + V_{1}(\chi, \tau)]^{2} d\tau - \\ + f_{V}(\chi) + \frac{vL}{D_{0}} V_{1}(\chi, \vartheta) - \int_{0}^{\vartheta} k_{I,V}(\chi, T) [\alpha_{2I} + I_{1}(\chi, \tau)] [\alpha_{2V} + V_{1}(\chi, \tau)]^{2} d\tau - \\ + f_{V}(\chi) + \frac{\partial}{\partial \chi} \int_{0}^{\vartheta} \Delta_{\Phi_{V}}(\chi, T) \frac{\partial \Phi_{1I}(\chi, \tau)}{\partial \chi} d\tau + \int_{0}^{\vartheta} k_{I}(\chi, T) I(\chi, \tau) d\tau \\ \begin{cases} \Phi_{2I}(\chi, \vartheta) = \frac{\partial}{\partial \chi} \int_{0}^{\vartheta} \Delta_{\Phi_{V}}(\chi, T) \frac{\partial \Phi_{1I}(\chi, \tau)}{\partial \chi} d\tau + \int_{0}^{\vartheta} k_{I}(\chi, T) I(\chi, \tau) d\tau \\ \Phi_{2V}(\chi, \vartheta) = \frac{\partial}{\partial \chi} \int_{0}^{\vartheta} \Delta_{\Phi_{V}}(\chi, T) \frac{\partial \Phi_{1V}(\chi, \tau)}{\partial \chi} d\tau + \int_{0}^{\vartheta} k_{V}(\chi, T) V(\chi, \vartheta) + \\ + f_{\Phi_{V}}(\chi) + \int_{0}^{\vartheta} k_{V,V}(\chi, T) V^{2}(\chi, \tau) d\tau + \int_{0}^{\vartheta} k_{V}(\chi, T) V(\chi, \tau) d\tau \end{cases}$$

$$(6e)$$

Average values of the considered second-order approximations of the considered concentrations could be calculated by using the following standard relation

$$\alpha_{2\rho} = \frac{1}{\Theta} \int_{0}^{\Theta_1} \left[\rho_2(\chi, \vartheta) - \rho_1(\chi, \vartheta) \right] d\chi d\vartheta.$$
⁽¹⁰⁾

Substitution of relations (1e), (4e), (6e) into relation (10) gives a possibility to obtain relations for the considered average values

$$\alpha_{2\rho} = \frac{vL - D_0}{D_0} \int_0^1 f_C(\chi) \, d\chi \,, \tag{1f}$$

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$$\alpha_{2I} = \frac{\sqrt{(e_I + f \,\alpha_{2V})^2 - 4d_I(h_I \alpha_{2V} - g_I) - e_I - f \,\alpha_{2V}}}{d_I}$$

$$\alpha_{2V} = \sqrt[3]{\sqrt{\frac{2o}{27l} - \frac{n^2}{9 \cdot 27l^2} - \frac{1}{4} \left(\frac{2n^3}{27l^3} - \frac{2no}{3l^2} + \frac{w}{l}\right)^2} - \frac{1}{2} \left(\frac{2n^3}{27l^3} - \frac{2no}{3l^2} + \frac{w}{l}\right)}{3l^2} - \frac{1}{2} \left(\frac{2n^3}{27l^3} - \frac{2no}{3l^2} + \frac{w}{l}\right)}{3l^2} - \frac{1}{4} \left(\frac{2n^3}{27l^3} - \frac{2no}{3l^2} + \frac{w}{l}\right)^2}{3l^2} + \frac{1}{2} \left(\frac{2n^3}{27l^3} - \frac{2no}{3l^2} + \frac{w}{l}\right) - \frac{m}{2l}.$$
(4f)

where
$$d_{\rho} = \int_{0}^{\theta} \left(1 - \frac{g}{\Theta} \right)_{0}^{1} k_{\rho,\rho} (\chi, T) d\chi d\vartheta$$
, $e_{\rho} = 1 + 2 \int_{0}^{\theta} \left(1 - \frac{g}{\Theta} \right)_{0}^{1} k_{\rho,\rho} (\chi, T) I_{1} (\chi, \vartheta) d\chi d\vartheta$
+ $+ \int_{0}^{\theta} \left(1 - \frac{g}{\Theta} \right)_{0}^{1} k_{I,V} (\chi, T) V_{1} (\chi, \vartheta) d\chi d\vartheta$, $f = \int_{0}^{\theta} \left(1 - \frac{g}{\Theta} \right)_{0}^{1} k_{I,V} (\chi, T) d\chi d\vartheta$, $g_{\rho} = \alpha_{1,\rho} \frac{vL}{D_{0}} - \int_{0}^{\theta} \left(1 - \frac{g}{\Theta} \right)_{0}^{1} k_{\rho,\rho} (\chi, T) \rho_{1}^{2} (\chi, \vartheta) d\chi d\vartheta$, $f = \int_{0}^{\theta} \left(1 - \frac{g}{\Theta} \right)_{0}^{1} k_{I,V} (\chi, T) I_{1} (\chi, \vartheta) V_{1} (\chi, \vartheta) d\chi d\vartheta$
+ $+ \int_{0}^{1} f_{\rho} (\chi) d\chi$, $m = f^{2} d_{V} i - (f - 2d_{I}h_{I}) (2d_{V}f + d_{I}f)^{2} + f^{2} (2d_{V}f + d_{I}f) (2d_{V}e_{I} - d_{I}h_{V})$,
 $h_{\rho} = \int_{0}^{\theta} \left(1 - \frac{g}{\Theta} \right)_{0}^{1} k_{I,V} (\chi, T) \rho_{1} (\chi, \vartheta) d\chi d\vartheta$, $j = e_{I}^{2} d_{V} + d_{I} (4g_{I}d_{V} - e_{I}h_{V}) + d_{I}^{2} (e_{I}^{2} - g_{V})$,
 $i = 2e_{I}f d_{V} + e_{V} - f d_{I}h_{V} - 2e_{I}f d_{I}^{2} - 4h_{I}d_{I}d_{V} - d_{I}e_{I}f$, $l = f^{2} d_{V}^{2} - (2d_{V}f + d_{I}f)^{2} f^{2}$,
 $n = i^{2} - (2d_{V}f + d_{I}f)^{2} (e_{I}^{2} + 4d_{I}g_{I}) - f^{2} (2d_{V}e_{I} - d_{I}h_{V})^{2} (e_{I}^{2} + 4d_{I}g_{I}), o = (2d_{V}e_{I} - d_{I}h_{V}) + \times (2d_{V}e_{I} - d_{I}h_{V}) [(2d_{V}f + d_{I}f) (e_{I}^{2} + 4d_{I}g_{I}) - (f - 2d_{I}h_{I}) (2d_{V}e_{I} - d_{I}h_{V})] + i j$.
 $\langle 2d_{V}e_{I} - d_{I}h_{V} \rangle [(2d_{V}f + d_{I}f) (e_{I}^{2} + 4d_{I}g_{I}) - (f - 2d_{I}h_{I}) (2d_{V}e_{I} - d_{I}h_{V})] + i j$.
 $\langle 2d_{V}e_{I} - d_{I}h_{V} \rangle [(2d_{V}f + d_{I}f) (e_{I}^{2} + 4d_{I}g_{I}) - (f - 2d_{I}h_{I}) (2d_{V}e_{I} - d_{I}h_{V})] + i j$.
 $\langle 2d_{V}e_{I} - d_{I}h_{V} \rangle [(2d_{V}f + d_{I}f) (e_{I}^{2} + 4d_{I}g_{I}) - (f - 2d_{I}h_{I}) (2d_{V}e_{I} - d_{I}h_{V})] + i j$.
 $\langle 2d_{V}e_{I} = \frac{vL - D_{0}}{D_{0}} \alpha_{1\Phi_{V}} + \int_{0}^{\theta} \left(1 - \frac{g}{\Theta} \right)_{0}^{1} k_{V,V} (\chi, T) V^{2} (\chi, \theta) d\chi d\vartheta$
 $\langle 4g_{I} = \frac{vL - D_{0}}{D_{0}} \alpha_{1\Phi_{V}} + \int_{0}^{\theta} \left(1 - \frac{g}{\Theta} \right)_{0}^{1} k_{V} (\chi, T) V (\chi, \theta) d\chi d\vartheta$

In this paper the considered concentrations of dopant and radiation defects were calculated as the second-order approximations in the framework of method of averaging of function corrections. The approximation is usually enough adequate approximation to obtain qualitative conclusions and some quantitative results. Results of analytical calculations were checked by their comparison with results of numerical simulation.

3. DISCUSSION

In this section we analyzed redistribution of dopant and radiation defects in the considered multilayer structure. Fig. 2 shows distributions of concentrations of dopant at small speed of over-

growth. Increasing of number of curves corresponds to increasing of temperature. One can find similar curves at small value of continuance of overgrowth.

Fig. 3 shows distributions of concentrations of dopant at large speed of overgrowth. Increasing of number of curves corresponds to increasing of temperature. One can find similar curves at large value of continuance of overgrowth.



Fig. 2. Distributions of concentration of dopant at small speed of overgrowth. Increasing of number of curves corresponds to increasing of temperature. Distributions of concentration of dopant at small continuance of overgrowth are the similar to presented on this figure



Fig. 3. Distributions of concentration of dopant at large speed of overgrowth. Increasing of number of curves corresponds to increasing of temperature. Distributions of concentration of dopant at large continuance of overgrowth are the similar to presented on this figure

4. CONCLUSION

We analyzed redistribution of dopant in a multilayer structure during overgrowing of area doped by ion implantation. We analyzed the effect of changing of regimes of overgrowing of the doped area on the redistribution of dopant (changing of speed of overgrowth, changing of temperature

of overgrowth). We introduce an analytical approach for analysis of redistribution of dopant. The approach gives a possibility to simultaneously to take into account the changing of parameters of the considered process (diffusion coefficient of dopant and radiation defects, limit of solubility of dopant, parameters of interaction between radiation defects) in space (due to presents of several layers in the considered multilayer structure) and time (due to variation of temperature of overgrowth in time), as well as nonlinearity of the mass transport (due to interaction between radiation defects and dopant).

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