

RESEARCH ARTICLE

On Prognosis of Changing of the Rate of Diffusion of Radiation Defects, Generated during Ion Implantation, with Increasing of Depth of their Penetration

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ABSTRACT

In this paper, we introduce a model for the redistribution and interaction of point radiation defects between themselves, as well as their simplest complexes in a material, taking into account the experimentally non-monotonicity of the distribution of the concentration of radiation defects. To take into account this nonmonotonicity, the previously used model in the literature for the analysis of spatiotemporal distributions of the concentration of radiation defects was supplemented by the concentration dependence of their diffusion coefficient.

Key words: Analytical approach for modeling, ion implantation, model of radiation defects

INTRODUCTION

In the present time, the influence of different types of radiation processing on semiconductors is intensively analyzing.^[1-3] Based on the analysis, several recommendations to increase the radiation resistance have been formulated.^[4-6]

In this paper, we analyze redistribution and interaction between point radiation defects, as well as their simplest complexes in materials after ion implantation. A modification of the previously proposed model^[7] describing the redistribution and interaction of radiation defects between themselves is proposed with the aim of taking into account the experimentally revealed nonmonotonicity of the distribution of the concentrations of these defects.^[8]

METHOD OF SOLUTION

We determine spatiotemporal distributions of concentrations of point defects by the solution of the following system of equations.^[7,9]

$$\begin{cases} \frac{\partial I(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[D_I(I,V,T) \frac{\partial I(x,t)}{\partial x} \right] - K_I(T) I^2(x,t) - K_r(T) I(x,t) V(x,t) \\ \frac{\partial V(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[D_V(I,V,T) \frac{\partial V(x,t)}{\partial x} \right] - K_V(T) V^2(x,t) - K_r(T) I(x,t) V(x,t) \end{cases} \quad (1)$$

Here, $I(x, t)$ and $V(x, t)$ are the spatiotemporal distributions of concentrations of interstitials and vacancies. The first term in the right-hand side of Eqs. (1) describe the diffusion of point defects with the diffusion coefficient, which depends on temperature and concentration of point defects. The dependence

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could be approximated by the following relation $D_p(I, V, T) = D_0 [1 + a \times I(x, t)/I^* + b \times V(x, t)/V^*]$, $p = I, V$. The second term on the right-hand side of Eqs. (1) describes the generation of the simplest complexes of radiation defects (divacancies and analogous complexes of radiation defects).^[7] The third term on the right-hand side of Eqs. (1) describes the recombination of point defects.

$$\left. \frac{\partial I(x, t)}{\partial x} \right|_{x=0} = 0, \left. \frac{\partial V(x, t)}{\partial x} \right|_{x=0} = 0, \left. \frac{\partial I(x, t)}{\partial x} \right|_{x=L} = 0, \left. \frac{\partial V(x, t)}{\partial x} \right|_{x=L} = 0,$$

$$I(x, 0) = N_I \exp\left[-\frac{(x-x_{0I})^2}{x_I^2}\right], V(x, 0) = N_V \exp\left[-\frac{(x-x_{0V})^2}{x_V^2}\right]. \tag{2}$$

We transform Eqs. (1) to the following integral form,

$$\left\{ \begin{aligned} I(x, t) &= \frac{\partial}{\partial x} \left[\int_0^t D_I(T) \frac{\partial I(x, \tau)}{\partial x} d\tau \right] - \int_0^t K_I(T) I^2(x, \tau) d\tau - \\ &\quad - \int_0^t K_r(T) I(x, \tau) V(x, \tau) d\tau + I(x, 0) \\ V(x, t) &= \frac{\partial}{\partial x} \left[\int_0^t D_V(T) \frac{\partial V(x, \tau)}{\partial x} d\tau \right] - \int_0^t K_V(T) V^2(x, \tau) d\tau - \\ &\quad - \int_0^t K_r(T) I(x, \tau) V(x, \tau) d\tau + V(x, 0) \end{aligned} \right. \tag{1a}$$

Now, we will solve Eqs. (1a) by the method of averaging of function corrections,^[10] with decreasing quantity of iteration steps.^[11] We used solutions of Eqs. (1) without nonlinear terms and averaged diffusion coefficients D_{0I} as initial-order approximations of solutions of Eqs. (1a). These initial-order approximations could be solved by standard Fourier approach^[10,11] and could be written as:

$$I_0(r, z, t) = F_{0I} + \sum_{n=1}^{\infty} F_{nI} J_0\left(\frac{r}{R}\right) \cos\left(\frac{\pi n z}{L}\right) \exp\left(-\frac{\pi^2 n^2 D_{0I} t}{L^2}\right),$$

$$V_0(r, z, t) = F_{0V} + \sum_{n=1}^{\infty} F_{nV} J_0\left(\frac{r}{R}\right) \cos\left(\frac{\pi n z}{L}\right) \exp\left(-\frac{\pi^2 n^2 D_{0V} t}{L^2}\right).$$

Here $F_{nI} = \frac{2}{L} \int_0^L I(u, 0) \cos\left(\frac{\pi n u}{L}\right) du$, $F_{nV} = \frac{2}{L} \int_0^L V(u, 0) \cos\left(\frac{\pi n u}{L}\right) du$. Substitution of the above series into Eqs. (1a) gives us a possibility to obtain the first-order approximations of concentrations of point radiation defects in the following form:

$$I_1(x, t) = -\frac{\pi}{L} \sum_{n=1}^{\infty} n F_{nI} \sin\left(\frac{\pi n x}{L}\right) \left[\int_0^t D_I(T) \exp\left(-\frac{\pi^2 n^2 D_{0I} \tau}{L^2}\right) d\tau \right] - \int_0^t K_I(T) \left[\sum_{n=1}^{\infty} \cos\left(\frac{\pi n x}{L}\right) \right. \\ \times F_{nI} \exp\left(-\frac{\pi^2 n^2 D_{0I} \tau}{L^2}\right) + \frac{F_{0I}}{2} \left. \right]^2 d\tau - \int_0^t K_r(T) \left[\frac{F_{0I}}{2} + \sum_{n=1}^{\infty} F_{nI} \cos\left(\frac{\pi n x}{L}\right) \exp\left(-\frac{\pi^2 n^2 D_{0I} \tau}{L^2}\right) \right] \\ \times \left[\frac{F_{0V}}{2} + \sum_{n=1}^{\infty} F_{nV} \cos\left(\frac{\pi n x}{L}\right) \exp\left(-\frac{\pi^2 n^2 D_{0V} \tau}{L^2}\right) \right] d\tau + I(x, 0) \tag{1a}$$

$$\begin{aligned}
 V_1(x, t) = & -\frac{\pi}{L} \sum_{n=1}^{\infty} n F_{nV} \sin\left(\frac{\pi n x}{L}\right) \left[\int_0^t D_V(T) \exp\left(-\frac{\pi^2 n^2 D_{0V} \tau}{L^2}\right) d\tau \right] - \int_0^t K_V(T) \left[\sum_{n=1}^{\infty} \cos\left(\frac{\pi n x}{L}\right) \right. \\
 & \times F_{nV} \exp\left(-\frac{\pi^2 n^2 D_{0V} \tau}{L^2}\right) + \frac{F_{0V}}{2} \left. \right]^2 d\tau - \int_0^t K_r(T) \left[\frac{F_{0I}}{2} + \sum_{n=1}^{\infty} F_{nI} \cos\left(\frac{\pi n x}{L}\right) \exp\left(-\frac{\pi^2 n^2 D_{0I} \tau}{L^2}\right) \right] \\
 & \times \left[\frac{F_{0V}}{2} + \sum_{n=1}^{\infty} F_{nV} \cos\left(\frac{\pi n x}{L}\right) \exp\left(-\frac{\pi^2 n^2 D_{0V} \tau}{L^2}\right) \right] d\tau + V(x, 0)
 \end{aligned}$$

We determine the second and highest orders of approximations of concentrations of point radiation defects framework standard iterative procedure of method of averaging of function corrections.^[10] In this case, n th-order approximations of concentrations of defects will be determined by the following replacement $I(x, t) \rightarrow \alpha_{nI} + I_{n-1}(x, t)$, $V(x, t) \rightarrow \alpha_{nV} + V_{n-1}(x, t)$ in the right sides of Eqs. (1a), where α_{nI} and α_{nV} are the average values of the considered approximations. In this situation, the second-order approximations of concentrations of point defects could be written as:

$$\begin{cases}
 I_2(x, t) = \frac{\partial}{\partial x} \left[\int_0^t D_I(T) \frac{\partial I_1(x, \tau)}{\partial x} d\tau \right] - \int_0^t K_r(T) [\alpha_{2I} + I_1(x, \tau)] [\alpha_{2V} + V_1(x, \tau)] d\tau \\
 \quad - \int_0^t K_I(T) [\alpha_{2I} + I_1(x, \tau)]^2 d\tau + I(x, 0) \\
 V_2(x, t) = \frac{\partial}{\partial x} \left[\int_0^t D_V(T) \frac{\partial V_1(x, \tau)}{\partial x} d\tau \right] - \int_0^t K_r(T) [\alpha_{2I} + I_1(x, \tau)] [\alpha_{2V} + V_1(x, \tau)] d\tau \\
 \quad - \int_0^t K_V(T) [\alpha_{2V} + V_1(x, \tau)]^2 d\tau + V(x, 0)
 \end{cases}$$

Average values of the second-order approximations of the considered concentrations could be determined by the following standard relations:

$$\alpha_{2I} = \frac{1}{\Theta L} \int_0^{\Theta} \int_0^L [I_2(x, t) - I_1(x, t)] dx dt, \quad \alpha_{2V} = \frac{1}{\Theta L} \int_0^{\Theta} \int_0^L [V_2(x, t) - V_1(x, t)] dx dt.$$

Where Θ is the continuance of observation of the change in the concentration of defects with time. Substitution of the appropriate approximations of concentrations of point defects into above relations leads to the following relations:

$$\alpha_{2V} = -\frac{\alpha_{2I}^2 A_{I000} + \alpha_{2I} (2A_{I010} + A_{r101} + 1) + (A_{I010} + A_{r111} + A_{I120})}{(\alpha_{2I} A_{r100} + A_{r110})},$$

$$\alpha_{2I} = \sqrt[3]{\frac{1}{27} \left(\frac{B_2}{B_4} - \frac{B_3^2}{3B_4^2} \right)^3 - \frac{B_3^3}{27B_4^3} + \frac{B_2 B_3}{6B_4^2} - \frac{B_0}{2B_4}}$$

$$-\sqrt[3]{\frac{1}{27} \left(\frac{B_2}{B_4} - \frac{B_3^2}{3B_4^2} \right)^3 + \frac{B_3^3}{27B_4^3} - \frac{B_2 B_3}{6B_4^2} + \frac{B_0}{2B_4}}.$$

Here, $A_{\rhoijk} = \frac{1}{\Theta L} \int_0^{\Theta} (\Theta - t) \int_0^L K_{\rho}^i(T) I_1^j(x, t) V_1^k(x, t) dx dt$, $B_4 = A_{I000} (A_{I000} A_{V000} - A_{r100}^2)$, $B_3 = A_{I000}$

Now, we solve systems of Eqs. (3a) by the method of averaging of function corrections with decreasing quantity of iteration steps. We used solutions of Eqs. (3) without nonlinear terms and averaged diffusion coefficients D_{0IV} as initial-order approximations of solutions of Eqs. (3a). These initial-order approximations could be solved by standard Fourier approach and could be written as:

$$\Phi_{I0}(x, t) = \frac{F_{0\Phi_I}}{2} + \sum_{n=1}^{\infty} F_{n\Phi_I} \cos\left(\frac{\pi n x}{L}\right) \exp\left(-\frac{\pi^2 n^2 D_{0\Phi_I} t}{L^2}\right),$$

$$\Phi_{V0}(x, t) = \frac{F_{0\Phi_V}}{2} + \sum_{n=1}^{\infty} F_{n\Phi_V} \cos\left(\frac{\pi n x}{L}\right) \exp\left(-\frac{\pi^2 n^2 D_{0\Phi_V} t}{L^2}\right).$$

Here, $F_{n\Phi_I} = \frac{2}{L} \int_0^L \Phi_I(v, 0) \cos\left(\frac{\pi n v}{L}\right) dv$, $F_{n\Phi_V} = \frac{2}{L} \int_0^L \Phi_V(v, 0) \cos\left(\frac{\pi n v}{L}\right) dv$. Substitution of the above series into Eqs.(3a) gives us a possibility to obtain the first-order approximations of concentrations of point radiation defects in the following form:

$$\begin{aligned} \Phi_{I1}(x, t) = & -\frac{\pi}{L} \sum_{n=1}^{\infty} F_{n\Phi_I} \sin\left(\frac{\pi n x}{L}\right) \int_0^t D_{\Phi_I}(T) \exp\left(-\frac{\pi^2 n^2 D_{0\Phi_I} \tau}{L^2}\right) d\tau - \int_0^t k_I(T) \left[\frac{F_{0\Phi_I}}{2} + \sum_{n=1}^{\infty} F_{n\Phi_I} \right. \\ & \times \cos\left(\frac{\pi n x}{L}\right) \exp\left(-\frac{\pi^2 n^2 D_{0\Phi_I} \tau}{L^2}\right) \left. \right] d\tau + \int_0^t k_{I,I}(T) \left[\sum_{n=1}^{\infty} F_{n\Phi_I} \cos\left(\frac{\pi n x}{L}\right) \exp\left(-\frac{\pi^2 n^2 D_{0\Phi_I} \tau}{L^2}\right) \right. \\ & \left. + \frac{1}{2} F_{0\Phi_I} \right]^2 d\tau. \end{aligned}$$

$$\begin{aligned} \Phi_{V1}(x, t) = & -\frac{\pi}{L} \sum_{n=1}^{\infty} F_{n\Phi_V} \sin\left(\frac{\pi n x}{L}\right) \int_0^t D_{\Phi_V}(T) \exp\left(-\frac{\pi^2 n^2 D_{0\Phi_V} \tau}{L^2}\right) d\tau - \int_0^t k_V(T) \left[\frac{F_{0\Phi_V}}{2} + \sum_{n=1}^{\infty} F_{n\Phi_V} \right. \\ & \times \cos\left(\frac{\pi n x}{L}\right) \exp\left(-\frac{\pi^2 n^2 D_{0\Phi_V} \tau}{L^2}\right) \left. \right] d\tau + \int_0^t k_{V,V}(T) \left[\sum_{n=1}^{\infty} F_{n\Phi_V} \cos\left(\frac{\pi n x}{L}\right) \exp\left(-\frac{\pi^2 n^2 D_{0\Phi_V} \tau}{L^2}\right) \right. \\ & \left. + \frac{1}{2} F_{0\Phi_V} \right]^2 d\tau. \end{aligned}$$

We determine the second and highest orders of approximations of concentrations of simplest complexes of point radiation defects framework standard iterative procedure of method of averaging of function corrections.^[10] In this case, n th-order approximations of concentrations of complexes of defects will be determined by the following replacement: $\Phi_I(x, t) \rightarrow \alpha_{nI} + \Phi_{In-1}(x, t)$, $\Phi_V(x, t) \rightarrow \alpha_{nV} + \Phi_{Vn-1}(x, t)$ in the right sides of Eqs. (3a), where α_{nI} and α_{nV} are the average values of the considered approximations. In this situation, the second-order approximations of concentrations of complexes of point defects could be written as,

$$\begin{cases} \Phi_{2I}(x, t) = \frac{\partial}{\partial x} \int_0^t D_{\Phi_I}(T) \frac{\partial \Phi_{I1}(x, \tau)}{\partial x} d\tau + \int_0^t k_{I,I}(T) I^2(x, \tau) d\tau - \int_0^t k_I(T) I(x, \tau) d\tau + \Phi_I(x, 0) \\ \Phi_{2V}(x, t) = \frac{\partial}{\partial x} \int_0^t D_{\Phi_V}(T) \frac{\partial \Phi_{V1}(x, \tau)}{\partial x} d\tau + \int_0^t k_{V,V}(T) V^2(x, \tau) d\tau - \int_0^t k_V(T) V(x, \tau) d\tau + \Phi_V(x, 0) \end{cases}$$

We determine spatiotemporal distribution of temperature, generated during generation of radiation defects due to radiation processing, by the solution of the following equation:

$$c(T) \frac{\partial T(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[\lambda(T) \frac{\partial T(x,t)}{\partial x} \right]. \tag{5}$$

Temperature dependence of heat capacitance $c(T)$ could be approximated by the following function: $c(T) = c_0 [1 - \exp(-T/T_d)]$, where T_d is the Debye temperature. If current temperature is larger than the Debye temperature, heat conduction coefficient could be approximated by the following function: $\lambda(T) = \lambda_0 \{1 + \mu [T_d/T(x,t)]^\phi\}$. In the same area of temperatures, one can consider the following relation: $c(T) \approx c_0$. The Eq. (5) is complemented by the following boundary and initial conditions:

$$\left. \frac{\partial T(x,t)}{\partial x} \right|_{x=0} = 0, \quad \left. \frac{\partial T(x,t)}{\partial x} \right|_{x=L} = 0, \quad T(x,0) = T_r, \tag{6}$$

Here, T_r is the room temperature. With account dependence of heat diffusion coefficient on temperature, one can transform the Eq.(5) to the following differential (6a) or integral (6b) form:

$$\frac{c_0}{\phi} \frac{\partial T^\phi(x,t)}{\partial t} = \mu \lambda_0 T_d^\phi T(x,t) \frac{\partial^2 T(x,t)}{\partial x^2} - \mu \phi \lambda_0 T_d^\phi \left[\frac{\partial T(x,t)}{\partial x} \right]^2 \tag{7a}$$

$$\frac{c_0}{\phi} T^\phi(x,t) = \mu \lambda_0 T_d^\phi \int_0^t T(x,\tau) \frac{\partial^2 T(x,\tau)}{\partial x^2} d\tau - \mu \phi \lambda_0 T_d^\phi \int_0^t \left[\frac{\partial T(x,\tau)}{\partial x} \right]^2 d\tau. \tag{7b}$$

We solved the Eq. (6b) by method of averaging of function corrections with a decreased quantity of iterative steps. Framework the approach we used solutions of linear Eqs. (5) with averaged heat diffusion coefficients λ_0 as initial-order approximations of solutions of Eqs. (7b). These initial-order approximations could be solved by standard Fourier approach and could be written as:

$$T_0(x,t) = \frac{F_0}{2} + \sum_{n=1}^{\infty} F_n \cos\left(\frac{\pi n x}{L}\right) \exp\left(-\frac{\pi^2 n^2 \lambda_0 t}{L^2 c_0}\right).$$

Here, $F_n = \frac{2}{L} \int_0^L T(v,0) \cos\left(\frac{\pi n v}{L}\right) dv$. Substitution of the above series into Eqs. (7b) gives us a possibility to obtain the first-order approximation of temperature in the following form:

$$\begin{aligned} \frac{c_0}{\phi} T_1^\phi(x,t) = & -\mu \frac{\pi^2}{L^2} \int_0^t \left[\frac{F_0}{2} + \sum_{n=1}^{\infty} F_n \cos\left(\frac{\pi n x}{L}\right) \exp\left(-\frac{\pi^2 n^2 \lambda_0 \tau}{L^2 c_0}\right) \right] \sum_{n=1}^{\infty} \exp\left(-\frac{\pi^2 n^2 \lambda_0 \tau}{L^2 c_0}\right) d\tau \\ & \times n^2 F_n \cos\left(\frac{\pi n x}{L}\right) T_d^\phi - \mu \phi \lambda_0 T_d^\phi \frac{\pi^2}{L^2} \int_0^t \left[\sum_{n=1}^{\infty} n^2 F_n \sin\left(\frac{\pi n x}{L}\right) \exp\left(-\frac{\pi^2 n^2 \lambda_0 \tau}{L^2 c_0}\right) \frac{\partial T(x,\tau)}{\partial x} \right]^2 d\tau. \end{aligned}$$

We determine the second and highest orders of approximation of temperature framework standard iterative procedure of method of averaging of function corrections.^[10] In this case, n th-order approximation of temperature will be determined by following replacement: $T(x,t) \rightarrow \alpha_{nT} + T_{n-1}(x,t)$ in the right sides of Eqs. (7b), where α_{nT} is the average value of the considered approximation. In this situation, the second-order approximation of temperature could be written as:

$$T_2(x,t) = \left\{ \mu \lambda_0 T_d^\phi \frac{\phi}{c_0} \int_0^t [\alpha_{2T} + T_1(x,t)] \frac{\partial^2 T_1(x,\tau)}{\partial x^2} d\tau - \mu \lambda_0 T_d^\phi \frac{\phi^2}{c_0} \int_0^t \left[\frac{\partial T_1(x,\tau)}{\partial x} \right]^2 d\tau \right\}^{\frac{1}{\phi}}.$$

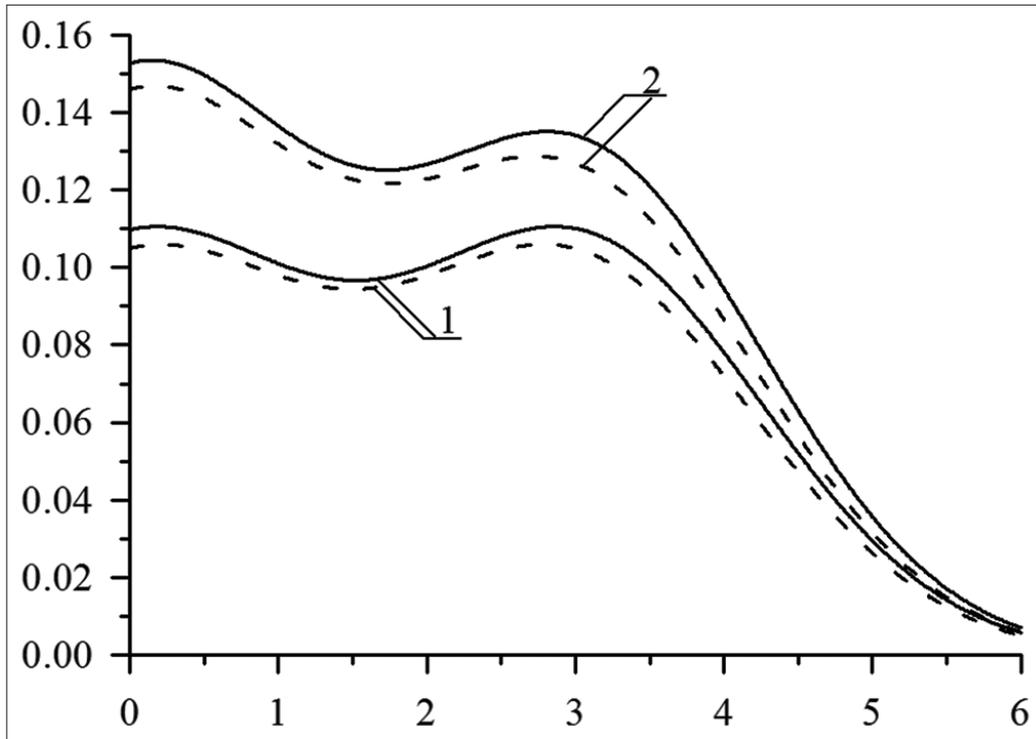


Figure 1: The distribution of the concentration of radiation defects at a dose $5 \times 10^{14} \text{ cm}^{-2}$ (curve 1) and a dose $5 \times 10^{15} \text{ cm}^{-2}$ (curve 2). Solid curves are the calculated results. Dotted curves are experimental results

Not yet known average value α_{2T} by solution the following equation:

$$\alpha_{2T} = \int_0^L \int_0^t \left\{ \mu \lambda_0 T_d^\phi \frac{\phi}{c_0} \int_0^t [\alpha_{2T} + T_1(x, \tau)] \frac{\partial^2 T_1(x, \tau)}{\partial x^2} d\tau - \mu \lambda_0 T_d^\phi \frac{\phi^2}{c_0} \int_0^t \left[\frac{\partial T_1(x, \tau)}{\partial x} \right]^2 d\tau \right\}^{\frac{1}{\phi}} - T_1(x, t) dx dt.$$

The value of this average value depends on the parameter Φ , determined by the experimental data.

DISCUSSION

In this paper, we analyzed spatiotemporal distribution of the concentrations of radiation defects in doped with ion implantation material. Figure 1 shows the distribution of the concentration of point radiation defects for two doses: $5 \times 10^{14} \text{ cm}^{-2}$ (curves 1) and $5 \times 10^{15} \text{ cm}^{-2}$ (curves 2). The solid lines are the calculated curves, and the dashed lines are the experimental curves.^[8] According to the experimental data, the concentration of defects increases to the irradiated sample boundary while having a maximum in the depth of the sample. Apparently, an increase in the concentration of defects with approach to the irradiated surface is a consequence of a large number of defects in the near-surface region at the initial stage of doping. Over time, the defects recombine among themselves and diffuse from the near-surface region. To account for these changes, the concentration dependence of the defect diffusion coefficient was used.

CONCLUSION

In this paper, we introduce a model for the redistribution and interaction of point radiation defects between themselves, as well as their simplest complexes in a material, taking into account the experimentally non-monotonicity of the distribution of the concentration of radiation defects. To take into account this non-monotonicity, the previously used model in the literature for the analysis of spatiotemporal distributions of the concentration of radiation defects was supplemented by the concentration dependence of their diffusion coefficient.

CONFLICTS OF INTERESTS

The authors declare that they have no conflicts of interest.

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