We calculate spatiotemporal distributions of dopant in an implanted-heterojunction rectifier. We analyzed the influence of inhomogeneity of heterostructure on dopant distribution. The influence of radiation processing of materials of the heterostructure, which has been done during ion implantation, on properties of the heterostructure has been also analyzed. It has been shown that radiation processing of materials of heterostructure leads to a decrease in mechanical stress in heterostructure. Our calculations have been done by using analytical approach, which gives us the possibility to obtain all results without joining solutions on all interfaces of heterostructure.

1. Introduction

In the present time one can find intensive development of devices of solid state electronic devices. One way to this development is increasing of frequency of switching of p-n-junctions [1–3]. To solve this problem it could be new search materials with higher charge carriers mobility [4–7]. Another way to decrease switching time is increasing sharpness of p-n-junctions [8, 9]. It has been recently shown that manufacturing diffusing- or implanted-junction rectifiers in a heterostructure ($H$) and optimization time of annealing of dopant and/or radiation defects give us possibility to increase sharpness of p-n-junctions [10–12]. It is known that in any $H$ one could find mechanical stress. The strain arising due to mismatch of lattice distance in layers of $H$ [13, 14]. Let us consider the following situation for simultaneous decreasing of mechanical stress and increasing of sharpness of p-n-junctions. We consider a $H$ with two layers, which consist of a substrate ($S$) and an epitaxial layer (EL), with known type of conductivity: n or p (see Figure 1). A dopant has been implanted in the $S$ through the EL. The dopant produces the type of conductivity of $S$, which reverses in comparison with type of conductivity of EL. In this situation we consider such conditions of implantation, under which major portion of dopant will be implanted in the $S$. Further annealing of radiation defects has been considered. The main aim of the present paper is to determine the conditions, under which the mechanical stress in the $H$ will be decreased and at the same time sharpness of the p-n-junction will be increased.

2. Method of Solution

To solve our aims let us determine spatiotemporal distribution of dopant. We determine the distribution by solving the second Fick’s law [1–3]

$$
\frac{\partial C(\vec{r}, t)}{\partial t} = \nabla \left[ D_C \nabla [C(\vec{r}, t)] \right] + \Omega \nabla \int_0^{L_z} \mu(\vec{r}, t) C(\vec{r}, t) dz
$$

(1)
with boundary and initial conditions
\[
\frac{\partial C(\vec{r}, t)}{\partial x} \bigg|_{x=0} = 0, \quad \frac{\partial C(\vec{r}, t)}{\partial x} \bigg|_{x=L_x} = 0, \\
\frac{\partial C(\vec{r}, t)}{\partial y} \bigg|_{y=0} = 0, \quad \frac{\partial C(\vec{r}, t)}{\partial y} \bigg|_{y=L_y} = 0, \\
\frac{\partial C(\vec{r}, t)}{\partial z} \bigg|_{z=0} = 0, \quad \frac{\partial C(\vec{r}, t)}{\partial z} \bigg|_{z=L_z} = 0,
\]
\[ C(\vec{r}, 0) = f_C(\vec{r}). \]

Here \( C(\vec{r}, t) \) is the spatiotemporal distribution of dopant; \( \Omega \) is the atomic volume; symbols \( \nabla \) and \( \nabla_s \) denote volumetric and surface gradients; \( \vec{r} \) is the vector with components \( x, y, \) and \( z; \int_0^{L_z} C(\vec{r}, t) \, d z \) is the surface concentration of dopant on interface between layers of \( H; \mu(\vec{r}, t) \) is the chemical potential; \( D_C \) and \( D_{CS} \) are the coefficients of volumetric and surface diffusions, respectively. The first term of (2) describes the thermal diffusion of dopant. The second term of the equation describes the surficial diffusion under influence of mechanical stress. Values of the diffusion coefficients depend on properties of materials of layers of \( H \), rates of heating and cooling of \( H \) spatiotemporal distributions of dopant, and radiation defects. The dependence can be approximated by the following relations [2]:
\[
D_C = D_L(\vec{r}, T) \left[ 1 + \frac{\xi}{P^*} \frac{C(\vec{r}, t)}{P^*} \right] \times \left[ 1 + \xi_1 V(\vec{r}, t) \right] + \frac{V^2(\vec{r}, t)}{V^*} \right],
\]
\[
D_s = D_{SL}(\vec{r}, T) \left[ 1 + \frac{\xi_S}{P^*} \frac{C(\vec{r}, t)}{P^*} \right] \times \left[ 1 + \xi_1 V(\vec{r}, t) \right] + \frac{V^2(\vec{r}, t)}{V^*} \right].
\]

In the relations we used the following notations: \( D_L(\vec{r}, T) \) and \( D_{SL}(\vec{r}, T) \) are the spatial (due to inhomogeneity of heterostructure and radiation damage of materials) and temperature (due to Arrhenius law) dependence of dopant diffusion coefficients; \( T \) is the annealing temperature; \( P(\vec{r}, T) \) is the limit of solubility of dopant; parameter \( \gamma \) depends on properties of materials and could be integer in the following interval \( \gamma \in [1, 3] \) [17]; \( V(\vec{r}, t) \) is the spatiotemporal distribution of vacancies; \( V^* \) is the equilibrium distribution of vacancies. Dependence of dopant diffusion coefficients on concentration of dopant is discussed in detail in [17]. Dependence of dopant diffusion coefficients on concentrations of vacancies is generalization of analogous relation in [18]. The generalization accounting for the generation of di-vacancies. The generation accounting by quadratic terms of the approximation [19]. We determine spatiotemporal distributions of concentrations of radiation defects by solving the following system of equations [19, 20]:
\[
\frac{\partial R(\vec{r}, t)}{\partial t} = \nabla \left[ D_R(\vec{r}, T) \nabla \left[ R(\vec{r}, T) \right] \right] + \Omega \nabla S \left[ D_{RS} \nabla \mu(\vec{r}, T) \int_0^{L_z} R(\vec{r}, t) \, d z \right] - k_{RR}(\vec{r}, T) R^2(\vec{r}, t) - k_{I,V}(\vec{r}, T) I(\vec{r}, t) V(\vec{r}, t)
\]

with boundary and initial conditions
\[
\frac{\partial R(\vec{r}, t)}{\partial x} \bigg|_{x=0} = 0, \quad \frac{\partial R(\vec{r}, t)}{\partial x} \bigg|_{x=L_x} = 0, \\
\frac{\partial R(\vec{r}, t)}{\partial y} \bigg|_{y=0} = 0, \quad \frac{\partial R(\vec{r}, t)}{\partial y} \bigg|_{y=L_y} = 0, \\
\frac{\partial R(\vec{r}, t)}{\partial z} \bigg|_{z=0} = 0, \quad \frac{\partial R(\vec{r}, t)}{\partial z} \bigg|_{z=L_z} = 0,
\]
\[ R(\vec{r}, 0) = f_R(\vec{r}). \]

Here \( R \) is \( I \) or \( V; I(\vec{r}, t) \) is the spatiotemporal distribution of interstitials; \( I^* \) is the equilibrium distribution of interstitials; \( D_L(\vec{r}, T), D_{RS}(\vec{r}, T) \) are the volumetric and surface diffusion coefficients of interstitials and vacancies, respectively; \( k_{I,V}(\vec{r}, T) \), \( k_{I,V}(\vec{r}, T) \), and \( k_{I,V}(\vec{r}, T) \) are the parameters of recombination of point defects (first of them) and generation of their complexes, respectively. The first term of (4) describes the thermal diffusion of point radiation defects. The second term of the equations describes the surficial diffusion under influence of mechanical stress. Terms with \( V^2(\vec{r}, t) \) and \( I^2(\vec{r}, t) \) correspond to generation of divacancies and di-interstitials (see, e.g., [19] and appropriate references in the work). The last terms of the equations correspond to recombination of point defects.

We determined spatiotemporal distributions of concentrations of divacancies \( \Phi_V(\vec{r}, t) \) and di-interstitials \( \Phi_I(\vec{r}, t) \) as...
solution of the following system of equations [19–21]:

\[
\frac{\partial \Phi_R(\vec{r}, t)}{\partial t} = \nabla \left[ D_{\Phi_R}(\vec{r}, T) \nabla \Phi_R(\vec{r}, t) \right] - k_R(\vec{r}, T) R(\vec{r}, t)
\]

\[
+ k_{R,R}(\vec{r}, T) R^2(\vec{r}, t)
\]

with boundary and initial conditions

\[
\frac{\partial \Phi_R(\vec{r}, t)}{\partial x} \bigg|_{x=0} = 0, \quad \frac{\partial \Phi_R(\vec{r}, t)}{\partial x} \bigg|_{x=L_x} = 0,
\]

\[
\frac{\partial \Phi_R(\vec{r}, t)}{\partial y} \bigg|_{y=0} = 0, \quad \frac{\partial \Phi_R(\vec{r}, t)}{\partial y} \bigg|_{y=L_y} = 0,
\]

\[
\frac{\partial \Phi_R(\vec{r}, t)}{\partial z} \bigg|_{z=0} = 0, \quad \frac{\partial \Phi_R(\vec{r}, t)}{\partial z} \bigg|_{z=L_z} = 0,
\]

\[
\Phi_R(\vec{r}, 0) = f_{\Phi_R}(\vec{r}).
\]  

where \( \sigma(z) \) is Poisson coefficient; \( \epsilon_0 = (\alpha_s - \alpha_{EL})/\alpha_{EL} \) is the mismatch parameter; \( \alpha_s, \alpha_{EL} \) are lattice distances of S and EL; \( K(z) \) is the modulus of uniform compression; \( \beta(z) \) is the coefficient of thermal expansion; \( T_e \) is the equilibrium temperature, which coincides (for our case) with room temperature. Components of displacement vector could be obtained by solution of the following equations [22]:

\[
\rho(z) \frac{\partial^2 u_{ij}(\vec{r}, t)}{\partial t^2} = \sum_{j=1}^{3} \frac{\partial \sigma_{x_{ij}}(\vec{r}, t)}{\partial x_j},
\]

where \( \sigma_{x_{ij}} = \langle E(z)/2 \rangle \left[ 1 + \epsilon(z) \right] \left[ \frac{\partial u_{x_i}(\vec{r}, t) / \partial x_i + \partial u_{x_j}(\vec{r}, t) / \partial x_j - (\delta_{ij}/3) \partial u_{x_k}(\vec{r}, t) / \partial x_k \right] + K(z) \delta_{ij} \partial u_{x_i}(\vec{r}, t) / \partial x_k - \beta(z) \times K(z)[T(\vec{r}, t) - T_r]; i = 1, 3; x_i, x_j, x_k \) are the coordinate \( x, y, z; \rho(z) \) is the density of materials of \( H; \delta_{ij} \) is the Kronecker symbol. Taking into account the relation for \( \sigma_{x_{ij}} \) last system of equation could be written as

\[
\rho(z) \frac{\partial^2 u_{ij}(\vec{r}, t)}{\partial t^2} = \sum_{j=1}^{3} \frac{\partial \sigma_{x_{ij}}(\vec{r}, t)}{\partial x_j}.
\]

Conditions for the system of \( (11) \) could be written in the following form:

\[
\frac{\partial \vec{u}(\vec{r}, t)}{\partial x} \bigg|_{x=0} = 0; \quad \frac{\partial \vec{u}(\vec{r}, t)}{\partial x} \bigg|_{x=L_x} = 0;
\]

\[
\frac{\partial \vec{u}(\vec{r}, t)}{\partial y} \bigg|_{y=0} = 0; \quad \frac{\partial \vec{u}(\vec{r}, t)}{\partial y} \bigg|_{y=L_y} = 0;
\]

\[
\frac{\partial \vec{u}(\vec{r}, t)}{\partial z} \bigg|_{z=0} = 0; \quad \frac{\partial \vec{u}(\vec{r}, t)}{\partial z} \bigg|_{z=L_z} = 0;
\]

\[
\vec{u}(\vec{r}, t) \bigg|_{t \to \infty} = \vec{u}_0;
\]

where \( \vec{u}(\vec{r}, t) \) is the displacement vector, \( \vec{u}_0 = \vec{u}(\vec{r}, t) \to \infty \) is the initial displacement vector. First of all let us estimate components of displacement vector. To make this procedure we used method of averaging of function corrections [11, 12, 21, 23]. Let us previously transform the equations of the system (11) to the integro-differential form. The transformation is based on integration of the both sides of (11) on time \( t \). After that we determine both integration constants by using both appropriate conditions. Furthermore we made analogous procedure with...
integration on coordinate $z$. The main aim of this transformation is to remove derivative on coordinate $z$, because many parameters ($E(z), \sigma(z), K(z), \ldots$) depend on coordinate $z$. Differentiation of step-wise functions leads to unphysical results. At the same time we were forced to make integration of both sides of (11) on time $t$. It is necessary to calculate an approximate solution of (11). The necessity is more clear for calculation of concentrations of dopant and radiation defects. The obtained integrodifferential equations are bulky and as being due to have been removed into Appendix. Framework the approach we replace components of displacement vector $u_i(\vec{R}, t)$ in the right sides of integro-differential equations on their not yet known average values $\alpha_{u1}$, where $s = x, y, z$. The average values we determined as

$$\alpha_{u1} = \frac{1}{\Theta V} \int_0^\Theta \int_0^V \int_0^L u_{v1}(\vec{r}, t) \, dV \, dt,$$  

(13)

where $V = L_xL_yL_z$, $dV = dx \, dy \, dz$.

The replacement gives us the possibility to obtain the first-order approximation of the components of displacement vector as follows:

$$u_{a1}(\vec{r}, t) = \phi \left[ t \int_0^\infty \int_0^z K(w) \alpha(w) \frac{\partial T(\vec{r}, t)}{\partial s} \, dw \, d\tau \right. - \left. \int_0^t (t - \tau) \int_0^z K(w) \beta(w) \frac{\partial T(\vec{r}, t)}{\partial s} \, dw \, d\tau \right]$$

(14)

$$- \alpha_{u1} \Phi_{a0}(\vec{r}_i, t) + \alpha_{u1}.$$

Here $\vec{r}_i$ is the vector with components $x, y, z$; and $w/\phi = \sqrt{V/\Theta^2E_1}$; $E_0$ is the average value of Young modulus.

Substitution of the first-order approximations into relation (13) gives us the possibility to determine average values $\alpha_{u1}$. Simple mathematical transformations give us the average values in the following form:

$$\alpha_{u1} = \frac{\Omega \int L_z [X_{x0}(\alpha) - X_{x2}(\Theta)]}{8V \int L_z (L_z - z) \rho(z) \, dz},$$

(15)

where $X_{ji}(\Theta) = \int_0^\Theta (1 + t/\Theta)^{j-1} \int_0^L \int_0^z K(z) \chi(z) (\partial T(\vec{r}, t)/\partial s) \, dw \, d\tau \, dt \, dV$.

Approximation of components of displacement vector of the second-order $u_{a2}(\vec{r}, t)$ and approximation of the components with higher order $n$ (i.e., $u_{sn}(\vec{r}, t)$) could be calculated by replacement of the components in the following sums $\alpha_{u2} + u_{sn-1}(\vec{r}, t)$, where

$$\alpha_{u1} = \frac{1}{\Theta V} \int_0^\Theta \int_0^V \int_0^L [u_{sn}(\vec{r}, t) - u_{sn-1}(\vec{r}, t)] \, dV \, dt.$$  

(16)

Results of the replacement for $n = 2$ and results of calculations of the parameters $\alpha_{u2}$ are presented in the Appendix, because the parameters are bulky.

Furthermore we determine spatiotemporal distributions of concentrations of point radiation defects. To calculate the distributions we also used method of averaging of function corrections. In the framework of the approach we replace the concentrations $R(\vec{r}, t)$ on their average values $\alpha_{1R}$. After the replacement we obtained equations for the first-order approximations of concentrations of point radiation defects $R_i(\vec{r}, t)$

$$\frac{\partial R_i(\vec{r}, t)}{\partial t} = \alpha_{1R} \Omega L_z V [\frac{D_{gs} \psi_s}{kT} \mu(\vec{r}, t)]$$

$$- \alpha_{1R} \kappa_{1R}(\vec{r}, T) - \alpha_{1R} \alpha_{1V} \kappa_{1V}(\vec{r}, T).$$

Integration on time of the left and right sides of the above equations gives us the possibility to obtain the functions $R_i(\vec{r}, t)$, $R = I, V$ in the final form

$$R_i(\vec{r}, t) = \alpha_{1R} \Omega L_z V \left[ \frac{D_{gs} \psi_s}{kT} \mu(\vec{r}, t) \right]$$

$$- \alpha_{1R} \kappa_{1R}(\vec{r}, T) - \alpha_{1R} \alpha_{1V} \kappa_{1V}(\vec{r}, T).$$

Average values of the first-order approximations of concentrations of point radiation defects could be calculated by standard relation

$$\alpha_{1R} = \frac{1}{\Theta V} \int_0^\Theta \int_0^V \int_0^L R_i(\vec{r}, t) \, dV \, dt,$$

(19)

where $R = I, V$. Substitution of (16) into the relation (19) gives us the possibility to obtain the following equations for the average values $\alpha_{1R}$:

$$\alpha_{1R}B_{11}^{100} + \alpha_{1V}B_{1V}^{100} = \Omega A_{1R}^{00} + \Theta C_I - L_xL_yL_z \Theta,$$

$$\alpha_{1R}B_{1V}^{100} + \alpha_{1V}B_{1V}^{100} = \Omega A_{1V}^{00} + \Theta C_V - L_xL_yL_z \Theta,$$

(20)

where $A_{1R} = \Omega \int_0^\Theta (\Theta - \tau) \int_0^L \int_0^z \int_0^L \int_0^L R_i(\vec{r}, \tau) \, d\tau \, dw \, d\tau \, dt \, dV$; $C_R = \Omega \int_0^\Theta \int_0^L \int_0^L \int_0^L R_i(\vec{r}, \tau) \, d\tau \, dw \, d\tau \, dt \, dV$.

Solution of the system of equations is as follows:

$$\alpha_{1V} = \left[ A_{1V}^{00} - V\Theta - (A_{1V}^{00} + C_V - V\Theta) \right] \frac{B_{1V}^{00}}{B_{1V}^{00}} \times \left( B_{1V} + \frac{B_{1V}^{100}}{B_{1V}^{00}} \right),$$

$$\alpha_{1R} = \left[ A_{1R}^{00} + C_I - V\Theta \right] \frac{B_{1R}^{100}}{B_{1R}^{00}}.$$  

Approximations of the second and higher orders of concentrations of point radiation defects within the framework method of averaging of function corrections could
be obtained by using standard iteration procedure, that is, by replacing of the functions \( R(\bar{r},t) \) on the following sums \( \alpha_{nR} + R_{n-1}(\bar{r},t) \), where \( n \) is the order of approximation. In the present paper we consider only the second-order approximations of the functions \( R(\bar{r},t) \). The above substitution and integration on time of the left and right sides give us the possibility to obtain the second-order approximations of concentrations of defects \( R_2(\bar{r},t) \) in the following form:

\[
R_2(\bar{r},t) = \nabla V \left[ \int_0^t D_R(\bar{r},T) \nabla R_1(\bar{r},\tau) \, d\tau \right] \\
- \int_0^t k_{R,R}(\bar{r},\tau) \left[ \alpha_{2R} + R_1(\bar{r},\tau) \right]^2 \, d\tau \\
- \int_0^t k_{I,V}(\bar{r},\tau) \left[ \alpha_{2L} + I_1(\bar{r},\tau) \right] \, d\tau \\
\times \left[ \alpha_{2V} + V_1(\bar{r},\tau) \right] \, d\tau \\
+ \Omega V_S \left[ \int_0^t \frac{D_{RS}}{kT} V_{\bar{S} \bar{M}}(\bar{r},\tau) \right] \, d\tau \\
+ f_R(\bar{r}). \tag{22}
\]

Average values of the second-order approximation and approximations of the higher orders of concentrations of point radiation defects \( \alpha_{nR} \) could be calculated by using standard relation \([11, 12, 21, 23]\)

\[
\alpha_{2R} = \frac{1}{2} \int_0^\Theta \int_V \left[ R_n(\bar{r},t) - R_{n-1}(\bar{r},t) \right] \, dV \, dt. \tag{23}
\]

Substitution of the first- and second-order approximations of the functions \( R(\bar{r},t) \) into (23) gives us the possibility to obtain the equations for the average values \( \alpha_{2R} \)

\[
\alpha_{2R} V\Theta = \Omega \int_0^\Theta (\Theta - t) \int_V \left[ \frac{D_{RS}}{kT} V_{\bar{S} \bar{M}}(\bar{r},\tau) \right] \, dV \, dt \\
- \int_0^\Theta (\Theta - t) \int_V k_{I,V}(\bar{r},T) \left[ \alpha_{2L} + I_1(\bar{r},\tau) \right] \, dV \, dt \\
\times \left[ \alpha_{2V} + V_1(\bar{r},\tau) \right] \, dV \, dt \\
- \int_0^\Theta (\Theta - t) \int_V k_{R,R}(\bar{r},T) \times \left[ \alpha_{2R} + R_1(\bar{r},\tau) \right]^2 \, dV \, dt. \tag{24}
\]

Solution of the above system of equations could be written as

\[
\alpha_{2L} = \frac{1}{2} \left\{ \frac{1}{4} a_1 a_3 \right\} \left[ \frac{1}{4} \left( a_1 + a_3 \right)^2 - 4 \left[ y + \frac{(a_2 y - a_0)}{a_1 a_6} \right] \right\} ,
\]

\[
\alpha_{2V} = \left[ C_l - \alpha_{2L} \left( 2B_{1I}^{110} + L \cdot L \cdot L \cdot L \cdot \Theta - A_1^0 + B_{1I}^{110} \right) \right] \\
- B_{1I}^{120} - \alpha_{2L} - A_{1I} + B_{1V}^{110} \right] \\
\times \left( \alpha_{2L} B_{1I}^{110} + B_{1I}^{110} \right)^{-1}, \tag{25}
\]

where \( a_1 = B_{1V}^{110} \left( \frac{B_{1I}^{110}}{B_{1V}^{110}} \right)^2 - B_{1I}^{100} \left( \frac{B_{1V}^{110}}{B_{1I}^{110}} \right)^2, \]
\( a_2 = B_{1I}^{100} B_{1V}^{110} \left( 2B_{1I}^{110} + V \Theta - A_1^0 + B_{1I}^{110} \right) - B_{1I}^{100} \left( 2B_{1I}^{110} + V \Theta - A_1^0 + B_{1I}^{110} \right), \]
\( a_3 = B_{1I}^{100} \left( 2B_{1I}^{110} + V \Theta - A_1^0 + B_{1I}^{110} \right), \]
\( a_4 = B_{1I}^{100} \left( 2B_{1I}^{110} + V \Theta - A_1^0 + B_{1I}^{110} \right) + A_{1I} F_{1V}^{110} + B_{1V}^{110} - A_1^0 \left( 2B_{1I}^{110} + V \Theta - A_1^0 + B_{1I}^{110} \right) \times \left( B_{1V}^{110} + V \Theta - A_1^0 + B_{1I}^{110} \right) + A_{1I} F_{1V}^{110} + B_{1V}^{110} - A_1^0 \left( 2B_{1I}^{110} + V \Theta - A_1^0 + B_{1I}^{110} \right), \]
\( a_6 = -\sqrt{q + \frac{a_1^2}{a_4} - \frac{a_0}{a_1} + \frac{q}{a_4}}, \]
\( q = a_1^2/216a_4^2 - a_1(a_4 - a_4)/48a_4^2 + a_4/16a_4, \]
\( y = \sqrt{-q + \sqrt{q^2 + p^2}}, p = (24a_1 a_4)/13824a_4^2. \)

System of (6) we solve by using method of averaging of function corrections in the same form as for system of (4). Within the framework of the approach we replace the functions \( \Phi_R(\bar{r},t) \) in the right sides of (6) on their average values \( \alpha_{2R} \). After the replacement we obtain the equations for the first-order approximations of concentrations of simplest complexes of radiation defects \( \Phi_{1R}(\bar{r},t) \) in the following form:

\[
\frac{\partial \Phi_{1R}(\bar{r},t)}{\partial t} = \alpha_{1R} \Omega L_z V_S \left[ \frac{D_{RS}}{kT} V_{\bar{S} \bar{M}}(\bar{r},\tau) \right] \\
- k_R(\bar{r},T) R(\bar{r},t) + k_{R,R}(\bar{r},T) R^2(\bar{r},t). \tag{26}
\]
Integration of left and right parts of the equations on time gives us the possibility to obtain the first-order approximations of concentrations of divacancies and di-interstitials in the final form

\[
\Phi_{I} (\vec{r}, t) = \alpha_{I} \Omega L_{2} V \left[ \int_{0}^{t} \frac{D \Phi_{I} \nabla \mu (\vec{r}, \tau)}{kT} d\tau \right] - k_{R} (\vec{r}, T) R (\vec{r}, t) + k_{R,R} (\vec{r}, T) R^{2} (\vec{r}, t) + f_{\Phi_{a}} (\vec{r}).
\]  

(27)

Average values \( \alpha_{\Phi I} \) and of the first-order approximations of concentrations of divacancies and di-interstitials can be calculated by standard relation, which analogous to relations (16) and (23). By calculation we obtain the following result:

\[
\alpha_{\Phi I} = \frac{(\Theta F_{I} - E_{I}^{1} + E_{I}^{2})}{L_{2} (L_{x} L_{y} \Theta - D_{II}^{0})},
\]

\[
\alpha_{\Phi V} = \frac{(\Theta F_{V} - E_{V}^{1} + E_{V}^{2})}{L_{2} (L_{x} L_{y} \Theta - D_{IV}^{0})},
\]

(28)

where \( D_{II}^{j} = \Omega \int_{0}^{\Theta} (\Theta - t) \int_{0}^{\tau} \int_{V_{1}} \int_{V_{2}} (\Phi_{I} \nabla \mu / kT) V \Phi_{I} dV d\tau dt, E_{I}^{1} = \int_{0}^{\Theta} (\Theta - t) \int_{0}^{\tau} \int_{V_{1}} \int_{V_{2}} k_{R} (\vec{r}, T) R (\vec{r}, t) dV dt, E_{V}^{1} = \int_{0}^{\Theta} (\Theta - t) \int_{0}^{\tau} \int_{V_{1}} \int_{V_{2}} k_{R,R} (\vec{r}, T) R^{2} (\vec{r}, t) dV dt, F_{I} = \int_{0}^{\Theta} (\Theta - t) \int_{0}^{\tau} \int_{V_{1}} \int_{V_{2}} f_{\Phi_{a}} (\vec{r}) dV.

The second-order approximations of concentrations of divacancies and di-interstitials could be calculated by standard iteration procedure of method of averaging of function corrections. The approximations could be written as

\[
\Phi_{2R} (\vec{r}, t) = V \left[ \int_{0}^{t} D_{\Phi_{a}} (\vec{r}, T) V \Phi_{IR} (\vec{r}, \tau) d\tau \right] + \int_{0}^{t} k_{R,R} (\vec{r}, T) R^{2} (\vec{r}, \tau) d\tau + f_{\Phi_{a}} (\vec{r}) + \Omega V \left[ \frac{D \Phi_{a} \nabla \mu}{kT} \right] x \left[ \int_{0}^{t} V \Phi_{a} (\vec{r}, \tau) \right] \times \left[ \int_{0}^{t} \int_{0}^{\tau} \int_{0}^{\tau} \left[ \alpha_{2\Phi_{a}} + \Phi_{2R} (\vec{r}_{1}, \tau) \right] dw d\tau \right] - \int_{0}^{t} k_{R} (\vec{r}, T) R (\vec{r}, \tau) d\tau.
\]

(29)

Average values \( \alpha_{2\Phi R} \) can be determined by standard relation. The relation is similar with relations (16) and (23). Results of calculation of the average values could be written as

\[
\alpha_{2\Phi_{a}} = \frac{D_{II}^{1} + G_{I}^{1} + F_{RI} + E_{I}^{0} - \alpha_{1\Phi_{a}} V \Theta}{V \Theta - D_{II}^{0}},
\]

\[
\alpha_{2\Phi_{V}} = \frac{D_{IV}^{1} + G_{I}^{1} + F_{IV} + E_{V}^{0} - \alpha_{1\Phi_{V}} V \Theta}{V \Theta - D_{IV}^{0}},
\]

(30)

where \( G_{R}^{i} = \int_{0}^{\Theta} (\Theta - t) \int_{0}^{\tau} \int_{V_{1}} \int_{V_{2}} V \Phi_{a} (\vec{r}, T) V \Phi_{IR} (\vec{r}, t) \int_{V} \int_{V} dV dt.

We calculate the distribution of dopant concentration by the same approach, which was used to calculate distributions of concentrations of defects. The first-order approximation of dopant concentration could be written as

\[
C_{1} (\vec{r}, t) = \alpha_{1C} V \int_{0}^{t} D_{2L} (\vec{r}, T) \times \left[ 1 + \xi_{1} V (\vec{r}, \tau) + \xi_{2} V^{2} (\vec{r}, \tau) \right] \times \left[ 1 + \alpha_{1C} L_{2} \Omega + f_{C} (\vec{r}) \right] d\tau.
\]

(31)

\[
C_{1} (\vec{r}, t) = \alpha_{1C} V \left[ \int_{0}^{t} \frac{D_{II}^{0}}{kT} \right] \left[ 1 + \frac{\alpha_{1C} L_{2} \Omega}{P_{C} (\vec{r}, T)} \right] d\tau.
\]

\[
\alpha_{1C} = \alpha_{1C} H_{1}^{0} + C_{C}.
\]

(32)

where \( H_{1}^{i} = \Omega \int_{0}^{\Theta} (\Theta - t) \int_{0}^{\tau} \int_{V_{1}} \int_{V_{2}} \left[ (1 + \xi_{1} V (\vec{r}, t)/V^{*}) + \xi_{2} (V^{2} (\vec{r}, t)/V^{*^{2}}) \right] \left[ 1 + \xi_{1} (\alpha_{1C} + C_{1} (\vec{r}, T)) / P_{C} (\vec{r}, T) \right] dV dt.

The solution of the equation depends on value of parameter \( \gamma \).

We determine the second-order approximation of dopant concentration \( C_{2} (x, y, z, t) \) within the framework of the same approach, which has been used for calculation of the second-order approximations of concentrations of radiation defects.
After simple mathematical transformation we obtain the function $C_2(x, y, z, t)$ in the final form

$$C_2(\vec{r}, t) = V \left( \frac{\int_{0}^{t} \left[ 1 + \xi \left[ \frac{\alpha_{SC} + C_1(\vec{r}, \tau)}{p^y(\vec{r}, T)} \right] \right] \times \left[ 1 + \xi_1 \frac{V(\vec{r}, \tau)}{V^*} + \xi_2 \frac{V^2(\vec{r}, \tau)}{(V^*)^2} \right] \nabla C_1(\vec{r}, \tau) \times D_L(\vec{r}, T) d\tau \right) + \Omega V_S \int_{\Theta}^{\Phi} \left[ 1 + \xi \left[ \frac{\alpha_{SC} + C_1(\vec{r}, \tau)}{p^y(\vec{r}, T)} \right] \right] \times D_{SL}(\vec{r}, T) \frac{V_S d\tau}{kT} \times \int_{\Theta}^{\Phi} \left[ \alpha_{SC} + C_1(\vec{r}, \tau) \right] d\omega d\tau + f_C(\vec{r}_i).$$

(33)

We determine the parameter $\alpha_{SC}$ by standard relation, which is analogous to relations (16) and (23). Substitution of the second-order approximation of dopant concentration $C_2(\vec{r}, t)$ into appropriate relation and simple mathematical transformations leads to the following equation for the parameter $\alpha_{SC}$:

$$\alpha_{SC} = \alpha_{IC} + \frac{J_1^I + H_1^I + F_C}{V \Theta},$$

(34)

where $J_1^I = \Omega \int_{\Theta}^{\Phi} (\Theta - t) \int_{\Theta}^{\Phi} \int_{\Theta}^{\Phi} V_S \left[ 1 + \xi \left[ \frac{\alpha_{IC} + C_{i-1}(\vec{r}, t)}{p^y(\vec{r}, T)} \right] \right] \left[ 1 + \xi_1 \left( \frac{V(\vec{r}, \tau)}{V^*} \right) + \xi_2 \left( \frac{V^2(\vec{r}, \tau)}{(V^*)^2} \right) \right] D_L(\vec{r}, T) dV d\tau.$

Further we used the obtained approximations of components of displacement vector, radiation defects, and dopant concentrations. The obtained relations give us the possibility to analyze demonstratively relaxations of dopant and radiation defects concentrations and components of displacement vector. Using numerical approaches gives us the possibility to amend the obtained results. In this situation we used both analytical and numerical approaches to solve (1), (4), (6), and (11).

3. Discussion

In this paragraph we analyzed dynamics of redistribution of implanted dopant in a heterostructure accounting for dynamics of redistribution of point radiation defects, redistribution of simplest complexes of point radiation defects, and relaxation of mechanical stress in the heterostructure. Some calculated dopant distributions are presented in Figure 2.

Some of the distributions have been calculated for homogeneous sample, and other distributions have been calculated for heterostructure. The figure shows that inhomogeneity of the heterostructure leads to increasing sharpness of p-n-junctions and homogeneity of dopant distribution in area, which was enriched by the dopant. Both effects will be increased with increasing difference between values of diffusion coefficients of dopant in layers of $H$. Implantation of ion of dopant leads to radiation processing of materials of $H$. The radiation processing leads to a decrease in the mechanical stress in the $H$. Dependences of component of displacement vector $u_z$ on coordinate $z$ is presented in Figure 3. The coordinate $z$ is perpendicular to interface between layers of $H$ (see Figure 1). Figure 3 shows that the value of component of displacement vector $u_z$ decreases after radiation processing (such as ion implantation). Probably, reason of the decreasing is dislodging of several atoms from matrix of materials of $H$. The dislodging leads to generation of radiation vacancies. Farther one can obtain compacting of area of $H$ under influence of mechanical stress. Ulterior annealing leads to balancing of concentration of interstitials in $H$.

4. Conclusion

In this paper we introduce an approach to increase sharpness of implanted-junction rectifier in a heterostructure and at the same time to increase homogeneity of dopant distribution in area, enriched by the dopant. At the same time we introduce an approach to decrease value of mechanical stress in the heterostructure due to radiation processing of materials during ion implantation. As accompanying results it could be considered as an analytical approach to calculate spatiotem- poral distributions of dopant and radiation defects (point defects and their simplest complexes) concentrations, as well as relaxation of mechanical stress in heterostructure, which
Figure 3: Normalized dependence of displacement vector $u_z$ on coordinate $z$ for epitaxial layer before (curve 1) and after (curve 2) radiation processing.

was taken into account during calculation of distributions concentrations.

Appendix

Integrodifferential form of equations for components of displacement vector $\vec{u}(\vec{r}, t)$ is as follows:

$$u_x(\vec{r}, t)$$

$$= u_x(\vec{r}, t)$$

$$+ \frac{1}{6} \int_0^t (t - \tau) \int_0^z \left[ \frac{3}{2} \frac{\partial^2 u_x(\vec{r}_1, \tau)}{\partial x^2} - \frac{\partial^2 u_y(\vec{r}_1, \tau)}{\partial x \partial y} - \frac{\partial^2 u_z(\vec{r}_1, \tau)}{\partial x \partial w} \right] E(w) dw \frac{d\tau}{1 + \sigma(w)}$$

$$- \frac{1}{6} \int_0^\infty \int_0^z \left[ \frac{3}{2} \frac{\partial^2 u_x(\vec{r}_1, \tau)}{\partial x^2} - \frac{\partial^2 u_y(\vec{r}_1, \tau)}{\partial x \partial y} - \frac{\partial^2 u_z(\vec{r}_1, \tau)}{\partial x \partial w} \right] K(w) dw d\tau$$

$$+ \int_0^t (t - \tau) \int_0^z \left[ \frac{3}{2} \frac{\partial^2 u_x(\vec{r}_1, \tau)}{\partial x^2} + \frac{\partial^2 u_y(\vec{r}_1, \tau)}{\partial x \partial y} + \frac{\partial^2 u_z(\vec{r}_1, \tau)}{\partial x \partial w} \right] K(w) dw d\tau$$

$$u_y(\vec{r}, t)$$

$$= u_y(\vec{r}, t)$$

$$+ \frac{1}{2} \int_0^t (t - \tau) \int_0^z \left[ \frac{3}{2} \frac{\partial^2 u_y(\vec{r}_1, \tau)}{\partial x^2} + \frac{\partial^2 u_x(\vec{r}_1, \tau)}{\partial x \partial y} \right] \frac{E(w) dw}{1 + \sigma(w)} d\tau$$

$$+ \int_0^t (t - \tau) \int_0^z \left[ \frac{3}{2} \frac{\partial^2 u_y(\vec{r}_1, \tau)}{\partial x^2} + \frac{\partial^2 u_x(\vec{r}_1, \tau)}{\partial x \partial y} \right] E(w) dw d\tau$$

$$- \frac{1}{2} \int_0^\infty \int_0^z \left[ \frac{3}{2} \frac{\partial^2 u_y(\vec{r}_1, \tau)}{\partial x^2} + \frac{\partial^2 u_x(\vec{r}_1, \tau)}{\partial x \partial y} \right] K(w) dw d\tau$$

$$- \int_0^\infty \int_0^z \left[ \frac{3}{2} \frac{\partial^2 u_y(\vec{r}_1, \tau)}{\partial x^2} + \frac{\partial^2 u_x(\vec{r}_1, \tau)}{\partial x \partial y} \right] K(w) dw d\tau$$

$$+ \int_0^\infty \int_0^z \left[ \frac{3}{2} \frac{\partial^2 u_y(\vec{r}_1, \tau)}{\partial x^2} + \frac{\partial^2 u_x(\vec{r}_1, \tau)}{\partial x \partial y} \right] E(w) dw d\tau$$

$$- \frac{1}{2} \int_0^\infty \int_0^z \left[ \frac{3}{2} \frac{\partial^2 u_y(\vec{r}_1, \tau)}{\partial x^2} + \frac{\partial^2 u_x(\vec{r}_1, \tau)}{\partial x \partial y} \right] K(w) dw d\tau$$

$$- \int_0^\infty \int_0^z \left[ \frac{3}{2} \frac{\partial^2 u_y(\vec{r}_1, \tau)}{\partial x^2} + \frac{\partial^2 u_x(\vec{r}_1, \tau)}{\partial x \partial y} \right] K(w) dw d\tau$$

$$+ \frac{1}{2} \int_0^t (t - \tau) \int_0^z \left[ \frac{3}{2} \frac{\partial^2 u_y(\vec{r}_1, \tau)}{\partial x^2} + \frac{\partial^2 u_x(\vec{r}_1, \tau)}{\partial x \partial y} \right] \frac{E(w) dw}{1 + \sigma(w)} d\tau$$

$$+ \int_0^t (t - \tau) \int_0^z \left[ \frac{3}{2} \frac{\partial^2 u_y(\vec{r}_1, \tau)}{\partial x^2} + \frac{\partial^2 u_x(\vec{r}_1, \tau)}{\partial x \partial y} \right] E(w) dw d\tau.$$
\[ \begin{align*} 
- \frac{t}{2} \int_0^{\infty} \int_0^z \left[ \frac{\partial^2 u_z(\vec{r}_1, \tau)}{\partial x^2} + \frac{\partial^2 u_y(\vec{r}_1, \tau)}{\partial x \partial y} \right] \\
\times E(\omega) \, dw \, d\tau \\
- t \int_0^t (t - \tau) \int_0^\infty K(\omega) \beta(\omega) \frac{\partial T(\vec{r}_1, \tau)}{\partial y} \, dw \, d\tau \\
+ \frac{t}{6} \int_0^{\infty} \int_0^z \left[ \frac{\partial^2 u_z(\vec{r}_1, \tau)}{\partial x^2} - \frac{\partial^2 u_y(\vec{r}_1, \tau)}{\partial x \partial y} - \frac{\partial^2 u_z(\vec{r}_1, \tau)}{\partial x \partial \omega} \right] \times E(\omega) \, dw \, d\tau \\
- \frac{t}{6} \int_0^{\infty} \int_0^z \frac{\partial^2 u_x(\vec{r}_1, \tau)}{\partial y^2} \times E(\omega) \, dw \, d\tau
\end{align*} \]

The second-order approximations of components of displacement vector could be written as

\[ 
\begin{align*} 
u_z(\vec{r}, t) &= u_z(\vec{r}, t) \\
+ \Phi_1 \left\{ \frac{1}{2} \int_0^t (t - \tau) \int_0^z \left[ \frac{\partial^2 u_z(\vec{r}_1, \tau)}{\partial x^2} + \frac{\partial^2 u_y(\vec{r}_1, \tau)}{\partial x \partial y} \right] \\
\times E(\omega) \, dw \, d\tau - \frac{t}{2} \int_0^\infty \int_0^z \left[ \frac{\partial^2 u_z(\vec{r}_1, \tau)}{\partial x^2} + \frac{\partial^2 u_y(\vec{r}_1, \tau)}{\partial x \partial \omega} \right] \\
\times E(\omega) \, dw \, d\tau + \frac{1}{2} \int_0^t (t - \tau) \int_0^z \left[ \frac{\partial^2 u_z(\vec{r}_1, \tau)}{\partial y^2} + \frac{\partial^2 u_y(\vec{r}_1, \tau)}{\partial y \partial \omega} \right] \times E(\omega) \, dw \, d\tau \right\}
\end{align*} \]

where \( \Phi_2(\vec{r}, t) = \int_0^z \rho(\omega) u_z(\vec{r}_1, \tau) \, dw. \)
\begin{align*}
+ \int_0^t (t - \tau) \times \int_0^z K(w) \\
\quad \times \left[ \frac{\partial^2 u_{x1}(\vec{r}_1, \tau)}{\partial x^2} + \frac{\partial^2 u_{y1}(\vec{r}_1, \tau)}{\partial x \partial y} + \frac{\partial^3 u_{x1}(\vec{r}_1, \tau)}{\partial x \partial y \partial\omega} \right] dw d\tau \\
- \int_0^\infty \int_0^z \left[ \frac{\partial^2 u_{x1}(\vec{r}_1, \tau)}{\partial x^2} + \frac{\partial^2 u_{y1}(\vec{r}_1, \tau)}{\partial x \partial y} + \frac{\partial^3 u_{x1}(\vec{r}_1, \tau)}{\partial x \partial y \partial\omega} \right] K(w) dw d\tau t \\
+ \frac{1}{2} \int_0^t (t - \tau) \int_0^z \left[ \frac{\partial^2 u_{x1}(\vec{r}_1, \tau)}{\partial x \partial y} + \frac{\partial^2 u_{y1}(\vec{r}_1, \tau)}{\partial y^2} + \frac{\partial^3 u_{x1}(\vec{r}_1, \tau)}{\partial x \partial y \partial\omega} \right] E(w) dw d\tau \\
- \frac{1}{2} \int_0^t \int_0^z \left[ \frac{\partial^2 u_{x1}(\vec{r}_1, \tau)}{\partial x \partial y} + \frac{\partial^2 u_{y1}(\vec{r}_1, \tau)}{\partial y^2} + \frac{\partial^3 u_{x1}(\vec{r}_1, \tau)}{\partial x \partial y \partial\omega} \right] E(w) dw d\tau \\
+ \int_0^\infty \int_0^z \left[ \frac{\partial^2 u_{x1}(\vec{r}_1, \tau)}{\partial x \partial y} + \frac{\partial^2 u_{y1}(\vec{r}_1, \tau)}{\partial y^2} + \frac{\partial^3 u_{x1}(\vec{r}_1, \tau)}{\partial x \partial y \partial\omega} \right] E(w) dw d\tau \\
- \int_0^\infty \int_0^z \left[ \frac{\partial^2 u_{x1}(\vec{r}_1, \tau)}{\partial x \partial y} + \frac{\partial^2 u_{y1}(\vec{r}_1, \tau)}{\partial y^2} + \frac{\partial^3 u_{x1}(\vec{r}_1, \tau)}{\partial x \partial y \partial\omega} \right] E(w) dw d\tau \\
- \frac{t}{2} \int_0^\infty \int_0^z \left[ \frac{\partial^2 u_{x1}(\vec{r}_1, \tau)}{\partial x \partial y} + \frac{\partial^2 u_{y1}(\vec{r}_1, \tau)}{\partial y^2} + \frac{\partial^3 u_{x1}(\vec{r}_1, \tau)}{\partial x \partial y \partial\omega} \right] E(w) dw d\tau \\
+ \int_0^\infty \int_0^z \chi(w) K(w) \frac{\partial T(\vec{r}_1, \tau)}{\partial x} dw d\tau \\
- \int_0^t (t - \tau) \int_0^z \chi(w) K(w) \frac{\partial T(\vec{r}_1, \tau)}{\partial x} dw d\tau \\
- \int_0^t (t - \tau) \int_0^z K(w) \chi(w) \frac{\partial T(\vec{r}_1, \tau)}{\partial x} dw d\tau \\
- \int_0^t (t - \tau) \int_0^z \frac{\partial^2 u_{x1}(\vec{r}_1, \tau)}{\partial x^2} \rho(w) dw d\tau \\
- \alpha_{wx2} \Phi_{x0}(\vec{r}, t)
\end{align*}
\[ u_{z2}(\vec{r},t) = \alpha_{z2} + u_{z1}(\vec{r},t) \]

\[ = \frac{1}{2} \int_0^t \left( t - \tau \right) \int_0^z \rho (w) \frac{\partial^2 u_{z1}(\vec{r}, \tau)}{\partial x^2} + \frac{\partial^2 u_{z1}(\vec{r}, \tau)}{\partial y \partial w} \left( \Theta - \tau \right) d\tau \frac{E (w)}{1 + \sigma (w)} dw d\tau \]

\[ - \frac{t}{2} \int_0^z \rho (w) \left( \frac{\partial^2 u_{z1}(\vec{r}, \tau)}{\partial x^2} + \frac{\partial^2 u_{z1}(\vec{r}, \tau)}{\partial y \partial w} \right) \left( \Theta - \tau \right) d\tau \frac{E (w)}{1 + \sigma (w)} dw d\tau \]

\[ + \frac{1}{2} \int_0^z \rho (w) \frac{\partial^2 u_{z1}(\vec{r}, \tau)}{\partial y^2} + \frac{\partial^2 u_{z1}(\vec{r}, \tau)}{\partial y \partial w} \frac{E (w)}{1 + \sigma (w)} dw d\tau \]

\[ - \int_0^z \rho (w) \frac{\partial T(\vec{r}, \tau)}{\partial w} K(w) \chi(w) d\tau d\tau \]

\[ - \frac{t}{2} \int_0^z \rho (w) \left( \frac{\partial^2 u_{z1}(\vec{r}, \tau)}{\partial x^2} + \frac{\partial^2 u_{z1}(\vec{r}, \tau)}{\partial y \partial w} \right) \frac{E (w)}{1 + \sigma (w)} dw d\tau \]

\[ + \frac{E (z)}{1 + \sigma (z)} \]

\[ \times \int_0^z \frac{\partial^2 u_{z1}(\vec{r}, \tau)}{\partial x^2} + \frac{\partial^2 u_{z1}(\vec{r}, \tau)}{\partial y \partial w} \frac{E (w)}{1 + \sigma (w)} dw d\tau \]

\[ - \frac{E (z)}{1 + \sigma (z)} \]

\[ + \frac{1}{2} \int_0^z \rho (w) \frac{\partial T(\vec{r}, \tau)}{\partial w} K(w) \chi(w) d\tau d\tau \]

\[ + \frac{E (z)}{1 + \sigma (z)} \]

\[ \times \int_0^z \frac{\partial^2 u_{z1}(\vec{r}, \tau)}{\partial x^2} + \frac{\partial^2 u_{z1}(\vec{r}, \tau)}{\partial y \partial w} \frac{E (w)}{1 + \sigma (w)} dw d\tau \]

\[ - \frac{E (z)}{1 + \sigma (z)} \]

\[ + \frac{1}{2} \int_0^z \rho (w) \frac{\partial T(\vec{r}, \tau)}{\partial w} K(w) \chi(w) d\tau d\tau \]

\[ + \frac{E (z)}{1 + \sigma (z)} \]

\[ \times \int_0^z \frac{\partial^2 u_{z1}(\vec{r}, \tau)}{\partial x^2} + \frac{\partial^2 u_{z1}(\vec{r}, \tau)}{\partial y \partial w} \frac{E (w)}{1 + \sigma (w)} dw d\tau \]

\[ - \frac{E (z)}{1 + \sigma (z)} \]

\[ + \frac{1}{2} \int_0^z \rho (w) \frac{\partial T(\vec{r}, \tau)}{\partial w} K(w) \chi(w) d\tau d\tau \]

\[ + \frac{E (z)}{1 + \sigma (z)} \]

\[ \times \int_0^z \frac{\partial^2 u_{z1}(\vec{r}, \tau)}{\partial x^2} + \frac{\partial^2 u_{z1}(\vec{r}, \tau)}{\partial y \partial w} \frac{E (w)}{1 + \sigma (w)} dw d\tau \]

\[ - \frac{E (z)}{1 + \sigma (z)} \]

\[ + \frac{1}{2} \int_0^z \rho (w) \frac{\partial T(\vec{r}, \tau)}{\partial w} K(w) \chi(w) d\tau d\tau \]

\[ + \frac{E (z)}{1 + \sigma (z)} \]

\[ \times \int_0^z \frac{\partial^2 u_{z1}(\vec{r}, \tau)}{\partial x^2} + \frac{\partial^2 u_{z1}(\vec{r}, \tau)}{\partial y \partial w} \frac{E (w)}{1 + \sigma (w)} dw d\tau \]
\[-\frac{\Theta^2}{2} \int_0^{\infty} \int_0^\infty \int_0^\infty V (L_z - z) K(z) \times \left[ \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial x^2} + \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial x \partial y} + \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial z^2} \right] dV dt + \frac{1}{2} \int_0^\Theta \int_0^\infty \int_0^\infty E(z) (L_z - z) \times \left[ \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial x^2} + \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial x \partial y} \right] dV dt \]

\[-\frac{\Theta^2}{2} \int_0^{\infty} \int_0^\infty \int_0^\Theta V (L_z - z) \times \left[ \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial x \partial y} + \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial z^2} \right] dV dt \]

\[-\frac{\Theta^2}{4} \int_0^{\Theta} \int_0^{L_z - z} (1 + \sigma(z)) \times \left[ \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial x \partial y} + \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial z^2} \right] dV dt + \frac{1}{2} \int_0^{\Theta} \int_0^{L_z - z} \rho(z) \times \left[ \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial x \partial y} + \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial z^2} \right] dV dt \]

\[-\frac{\Theta^2}{2} \int_0^{\infty} \int_0^\infty \int_0^{\Theta} V (L_z - z) \times \left[ \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial x \partial y} + \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial z^2} \right] dV dt + \frac{1}{2} \int_0^{\Theta} \int_0^{L_z - z} \rho(z) \left[ \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial x \partial y} + \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial z^2} \right] dV dt \]

\[-\frac{\Theta^2}{2} \int_0^{\Theta} \int_0^{L_z - z} \rho(z) \left[ \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial x \partial y} + \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial z^2} \right] dV dt \]

\[-\frac{\Theta^2}{2} \int_0^{\Theta} \int_0^{L_z - z} \rho(z) \left[ \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial x \partial y} + \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial z^2} \right] dV dt \]

\[-\frac{\Theta^2}{2} \int_0^{\Theta} \int_0^{L_z - z} \rho(z) \left[ \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial x \partial y} + \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial z^2} \right] dV dt \]

\[-\frac{\Theta^2}{2} \int_0^{\Theta} \int_0^{L_z - z} \rho(z) \left[ \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial x \partial y} + \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial z^2} \right] dV dt \]

\[-\frac{\Theta^2}{2} \int_0^{\Theta} \int_0^{L_z - z} \rho(z) \left[ \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial x \partial y} + \frac{\partial^3 u_{x1}(\vec{r}, t)}{\partial z^2} \right] dV dt \]
\[ -\frac{\Theta^2}{2} \int_0^\infty \int_0^{L_z} E(z) \left( \int_0^{L_z-z} \rho(z) u_{y_1}(\vec{r},t) \, dV \right) \, dV \, dt \]

\[ \frac{1}{2} \int_0^\infty \int_0^{L_z} \left[ \frac{\partial^2 u_{y_1}(\vec{r},t)}{\partial x^2} + \frac{\partial^2 u_{y_1}(\vec{r},t)}{\partial y \partial z} \right] E(z) \, dV \, dt \]

\[ -\frac{\Theta^2}{2} \int_0^\infty \int_0^{L_z} E(z) \left( \int_0^{L_z-z} \rho(z) u_{y_1}(\vec{r},t) \, dV \right) \, dV \, dt \]

\[ \frac{1}{2} \int_0^\infty \int_0^{L_z} \left[ \frac{\partial^2 u_{y_1}(\vec{r},t)}{\partial x^2} + \frac{\partial^2 u_{y_1}(\vec{r},t)}{\partial y \partial z} \right] E(z) \, dV \, dt \]

\[ \alpha_{\text{mc}} = L_z \left[ \frac{1}{2} \int_0^\infty (\Theta - t)^2 \right] \]

\[ \times \int_0^{L_z} E(z) \left( \int_0^{L_z-z} \rho(z) u_{y_1}(\vec{r},t) \, dV \right) \, dV \, dt \]

\[ \frac{1}{2} \int_0^\infty \int_0^{L_z} \left[ \frac{\partial^2 u_{y_1}(\vec{r},t)}{\partial x^2} + \frac{\partial^2 u_{y_1}(\vec{r},t)}{\partial y \partial z} \right] \, dV (\Theta - t)^2 \]

\[ -\frac{\Theta^2}{2} \int_0^\infty \int_0^{L_z} E(z) \left( \int_0^{L_z-z} \rho(z) u_{y_1}(\vec{r},t) \, dV \right) \, dV \, dt \]

\[ \frac{1}{2} \int_0^\infty \int_0^{L_z} \left[ \frac{\partial^2 u_{y_1}(\vec{r},t)}{\partial x^2} + \frac{\partial^2 u_{y_1}(\vec{r},t)}{\partial y \partial z} \right] E(z) \, dV \, dt \]

\[ -\frac{\Theta^2}{2} \int_0^\infty \int_0^{L_z} \left[ \frac{\partial^2 u_{y_1}(\vec{r},t)}{\partial x^2} + \frac{\partial^2 u_{y_1}(\vec{r},t)}{\partial y \partial z} \right] \, dV (\Theta - t)^2 \]

\[ \times \int_0^{L_z} E(z) \left( \int_0^{L_z-z} \rho(z) u_{y_1}(\vec{r},t) \, dV \right) \, dV \, dt \]

\[ \frac{1}{2} \int_0^\infty \int_0^{L_z} \left[ \frac{\partial^2 u_{y_1}(\vec{r},t)}{\partial x^2} + \frac{\partial^2 u_{y_1}(\vec{r},t)}{\partial y \partial z} \right] E(z) \, dV \, dt \]

\[ \left( A.5 \right) \]

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**References**


