Decreasing of quantity of radiation defects in an implanted-junction rectifiers by using overlayers

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Abstract
We introduce an approach to decrease quantity of radiation defects in area of implanted-heterojunction rectifier. The approach based on implantation of ions of dopant in a homogenous sample, overgrowth of the damaged area and annealing of radiation defects. In this situation under spatial conditions one can obtain decreasing of quantity of radiation defects.

1. INTRODUCTION

In the present time intensive refinement of element of integrated circuits and their discrete analogs (*p*-*n*-junctions and their systems: transistors and thyristors) is occurring. A problem of the refinement is manufacturing of structures with minimal quantity of defects. One way to manufacture of *p*-*n*-junctions is implantation of ions of dopant in homogenous sample or epitaxial layer (EL) [1-5]. During the ion implantation and other types of radiation processing [1-7] one can find generation of radiation defects in the processed samples. To decrease quantity of radiation defects it has been used or introduced some approaches [1-10]. Framework the paper we consider an approach to shift *p*-*n*-junction from the damaged area of the doped material. Let us consider a sample, which has been doped by ion implantation (Fig. 1). After implantation of ions of dopant an epitaxial layer has been grown under special conditions. Main aim of the present paper is analysis of influence of the overlayer (OL) on distribution of concentration of radiation defects.

2. METHOD OF SOLUTION

To solve our aim we determine spatiotemporal distributions of dopant and radiation defects. Spatiotemporal distribution of dopant we determined by solution of the second Fick's law

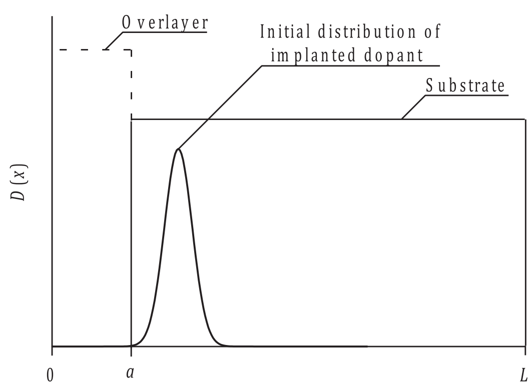

Fig. 1. Heterostructure with initial sample, overlayer and initial distribution of implanted dopant before starting of annealing of radiation defects

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

with boundary and initial conditions

$$\left.\frac{\partial C(x,t)}{\partial x}\right|_{x=0}=\left.\frac{\partial C(x,t)}{\partial x}\right|_{x=L}=0,\ C(x,0)=f_C(x). \tag{2}$$

Here $C(x,t)$ is the spatiotemporal distribution of concentration of dopant; D_C is the dopant diffusion coefficient. Value of dopant diffusion coefficient depends on properties of materials of heterostructure, velocity of heating and cooling (see Arrhenius law) and spatiotemporal distribution of concentration of dopant and radiation defects. Two last dependences of dopant diffusion coefficients could be approximated by the following relation [2,4,5]

$$D_C=D_L(x,T)\left[1+\xi\frac{C^\gamma(x,t)}{P^\gamma(x,T)}\right]\left[1+\varsigma\frac{V(x,t)}{V^*}\right]. \tag{3}$$

Here $D_L(x,T)$ is the spatial (due to inhomogeneity of heterostructure) and temperature (due to Arrhenius law, where T is the temperature) dependences of diffusion coefficient; $V(x,t)$ is the spatiotemporal distribution of concentration of radiation vacancies; V^* is the equilibrium distribution of vacancies; $P(x,T)$ is the limit of solubility of dopant; parameter g depends on properties of materials and could be equal values in the interval $\gamma\in[1,3]$ [2]. Concentrational dependence of dopant diffusion coefficient has been discussed in details in [2]. We determined spatiotemporal distributions of radiation defects from the following systems of equations [7,11]

$$\begin{cases}\dfrac{\partial I(x,t)}{\partial t}=\dfrac{\partial}{\partial x}\left[D_I(x,T)\dfrac{\partial I(x,t)}{\partial x}\right]-k_{I,V}(x,T)I(x,t)V(x,t)-k_{I,I}(x,T)I^2(x,t)\\[2ex] \dfrac{\partial V(x,t)}{\partial t}=\dfrac{\partial}{\partial x}\left[D_V(x,T)\dfrac{\partial V(x,t)}{\partial x}\right]-k_{I,V}(x,T)I(x,t)V(x,t)-k_{V,V}(x,T)V^2(x,t)\end{cases} \tag{4}$$

with boundary and initial conditions

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

Here $\rho = I,V$; $I(x,t)$ is the spatiotemporal distribution of concentration of interstitials; $D_\rho(x,T)$ are diffusion coefficients of interstitials and vacancies; $k_{I,V}(x,T)$ is the parameter of recombination; terms $V^2(x,t)$ and $I^2(x,t)$ correspond to generation of divacancies and analogous complexes of interstitials (see, for example, [12] and appropriate references in this work); $k_{I,V}(x,T)$, $k_{I,I}(x,T)$ and $k_{V,V}(x,T)$ are parameters of recombination of point defects and generation of their complexes. It could be take into account generation another complexes of radiation defects (complexes with three or larger vacancies or interstitials). But probability of generation of their complexes is smaller, than probability of generation of divacancies and diinterstitials.

Farther we determine spatiotemporal distributions of concentrations of divacancies F_V (x,t) and analogous complexes of interstitials F_I (x,t) by solving the following systems of equations [11,12]

$$\begin{cases} \dfrac{\partial \Phi_I(x,t)}{\partial t} = \dfrac{\partial}{\partial x}\left[D_{\Phi I}(x,T)\dfrac{\partial \Phi_I(x,t)}{\partial x}\right] + k_{I,I}(x,T)\, I^2(x,t) - k_I(x,T)\, I(x,t) \\ \dfrac{\partial \Phi_V(x,t)}{\partial t} = \dfrac{\partial}{\partial x}\left[D_{\Phi V}(x,T)\dfrac{\partial \Phi_V(x,t)}{\partial x}\right] + k_{V,V}(x,T)\, V^2(x,t) - k_V(x,T)\, V(x,t) \end{cases} \tag{6}$$

with boundary and initial conditions

$$\left.\frac{\partial \Phi_\rho(x,t)}{\partial x}\right|_{x=0} = \left.\frac{\partial \Phi_\rho(x,t)}{\partial x}\right|_{x=L} = 0\,,\ \Phi_r\,(x,0)=f_{Fr}\,(x). \tag{7}$$

Here $D_{\Phi I}(x,T)$ and $D_{\Phi V}(x,T)$ are the diffusion coefficients of complexes of point defects; $k_I(x, T)$ and $k_V(x,T)$ are decay parameters of complexes of point defects.

To determine spatiotemporal distributions of concentrations of radiation defects in pursuance of [13-15] we transform approximations of diffusion coefficients of points defects in the following form: $D_\rho(x,T)=D_{0\rho}[1+\varepsilon_\rho g_\rho(x,T)]$, where $D_{0\rho}$ is the average values of diffusion coefficients. We used analogous transformation of approximations of parameters of recombination of point radiation defects and generation of their complexes: $k_{I,V}(x,T)=k_{0I,V}[1+\varepsilon_{I,V}\, g_{I,V}(x,T)]$, $k_{I,I}(x,T)=k_{0I,I}[1+\varepsilon_{I,I}\, g_{I,I}(x,T)]$ and $k_{V,V}(x,T)= k_{0V,V}\, [1+\varepsilon_{V,V}\, g_{V,V}(x,T)]$, where $k_{0\rho 1,r2}$ are appropriate average values. Let us introduce the following dimensionless values: $\tilde{I}(x,t)=I(x,t)/I^*$, $\tilde{V}(x,t)=V(x,t)/V^*$, $\chi =x/L_x$, $\eta = y/L_y$, $\phi = z/L_z$, $\vartheta=\sqrt{D_{0I}D_{0V}}\,t/L^2$, $\omega=L^2k_{0I,V}\big/\sqrt{D_{0I}D_{0V}}$, $\Omega_\rho=L^2k_{0\rho,\rho}\big/\sqrt{D_{0I}D_{0V}}$. The introduction leads to transformation of Eqs.(4) and conditions (5)

$$\begin{cases} \dfrac{\partial \tilde{I}(\chi,\vartheta)}{\partial\vartheta} = \dfrac{D_{0I}}{\sqrt{D_{0I}D_{0V}}}\dfrac{\partial}{\partial\chi}\left\{\left[1+\varepsilon_I g_I(\chi,T)\right]\dfrac{\partial \tilde{I}(\chi,\vartheta)}{\partial\chi}\right\} - \\ \qquad -\omega\left[1+\varepsilon_{I,V}g_{I,V}(\chi,T)\right]\tilde{I}(\chi,\vartheta)\tilde{V}(\chi,\vartheta) - \Omega_I\left[1+\varepsilon_{I,I}g_{I,I}(\chi,T)\right]\tilde{I}^2(\chi,\vartheta) \\ \dfrac{\partial \tilde{V}(\chi,\vartheta)}{\partial\vartheta} = \dfrac{D_{0V}}{\sqrt{D_{0I}D_{0V}}}\dfrac{\partial}{\partial\chi}\left\{\left[1+\varepsilon_V g_V(\chi,T)\right]\dfrac{\partial \tilde{V}(\chi,\vartheta)}{\partial\chi}\right\} - \\ \qquad -\omega\left[1+\varepsilon_{I,V}g_{I,V}(\chi,T)\right]\tilde{I}(\chi,\vartheta)\tilde{V}(\chi,\vartheta) - \Omega_V\left[1+\varepsilon_{V,V}g_{V,V}(\chi,T)\right]\tilde{V}^2(\chi,\vartheta) \end{cases} \tag{8}$$

$$\left.\frac{\partial \tilde{\rho}(\chi,\vartheta)}{\partial\chi}\right|_{\chi=0} = \left.\frac{\partial \tilde{\rho}(\chi,\vartheta)}{\partial\chi}\right|_{\chi=1} = 0\,,\ \tilde{\rho}(\chi,\vartheta) = \frac{f_\rho(\chi,\vartheta)}{\rho^*}\,. \tag{9}$$

Solution of equation (8) with conditions (9) we determined in pursuance of works [13-15] as the following power series

$$\tilde{\rho}\left(\chi,\vartheta\right)=\sum_{i=0}^{\infty}\varepsilon_{\rho}^{i}\sum_{j=0}^{\infty}\omega^{j}\sum_{k=0}^{\infty}\Omega_{\rho}^{k}\tilde{\rho}_{ijk}\left(\chi,\vartheta\right). \tag{10}$$

Substitution the series (10) in the equations (8) and conditions (9) gives us possibility to obtain equations and conditions for initial approximations of concentrations of point defects $\tilde{I}_{000}\left(\chi,\vartheta\right)$ and $\tilde{V}_{000}\left(\chi,\vartheta\right)$ and corrections for them $\tilde{I}_{ijk}\left(\chi,\vartheta\right)$ and $\tilde{V}_{ijk}\left(\chi,\vartheta\right)$, $i \geq 1$, $j \geq 1$, $k \geq 1$. The equations and appropriate boundary and initial conditions are presented in the Appendix. Solutions of the equations could be determined by standard approaches (see, for example, [16,17]). Solutions of the equations with account boundary and initial conditions are presented in the Appendix. We obtain the second-order approximations of radiation point defects concentrations on all parameters ε_ρ, ω, Ω_ρ. The approximation could be used for all parameters within the following intervals $0\leq \varepsilon_\rho \sim 0.2$, $0\leq \omega \sim 0.2$, $0\leq \Omega_\rho \sim 0.2$.

Farther we determine spatiotemporal distributions of concentrations of complexes of point defects. To determine the distributions we transform the appropriate diffusion coefficients in the following form: $D_{Fr}(x,T)=D_{0Fr}[1+e_{Fr}g_{Fr}(x,T)]$, where D_{0Fr} are average values of diffusion coefficients. In this situation Eqs.(6) could be transformed in the form

$$\begin{cases}\dfrac{\partial\Phi_I\left(x,t\right)}{\partial t}=D_{0\Phi I}\dfrac{\partial}{\partial x}\left\{\left[1+\varepsilon_{\Phi I}g_{\Phi I}\left(x,T\right)\right]\dfrac{\partial\Phi_I\left(x,t\right)}{\partial x}\right\}+\\ \qquad\qquad+k_{I,I}\left(x,T\right)I^2\left(x,t\right)-k_I\left(x,T\right)I\left(x,t\right)\\ \dfrac{\partial\Phi_V\left(x,t\right)}{\partial t}=D_{0\Phi V}\dfrac{\partial}{\partial x}\left\{\left[1+\varepsilon_{\Phi V}g_{\Phi V}\left(x,T\right)\right]\dfrac{\partial\Phi_V\left(x,t\right)}{\partial x}\right\}+\\ \qquad\qquad+k_{V,V}\left(x,T\right)V^2\left(x,t\right)-k_V\left(x,T\right)V\left(x,t\right).\end{cases}$$

We determined solutions of these equations in the following form

$$\Phi_\rho\left(x,t\right)=\sum_{i=0}^{\infty}\varepsilon_{\Phi\rho}^{i}\Phi_{\rho i}\left(x,t\right). \tag{11}$$

Substitution the series (11) into the equations (6) and appropriate boundary and initial conditions gives us possibility to obtain equations for initial approximations of concentrations of complexes and corrections for them. The equations are presented in the Appendix. Appropriate conditions are presented in the Appendix. We obtain the second-order approximations of complexes of point defects concentrations on parameter $\varepsilon_{\Phi\rho}$. The approximation could be used for the parameter within the following interval $0\leq \varepsilon_{\Phi\rho} \sim 0.2$.

Spatiotemporal distribution of dopant concentration we determine by using the same approach as for solution of the previous equation. In this situation we transform approximation dopant diffusion coefficient in the following form: $D_L(x,T)=D_{0L}[1+ \varepsilon_L g_L(x,T)]$. In this situation we determine solution of the Eq.(1) in the following form

$$C\left(x,t\right)=\sum_{i=0}^{\infty}\varepsilon_L^i\sum_{\xi=1}^{\infty}\xi^jC_{ij}\left(x,t\right).$$

Substitution the series in the Eq.(1) and conditions (2) gives us possibility to obtain equations for initial approximation of concentration of dopant distribution $C_{00}(x,t)$ and correction for them $C_{ij}(x,t)$. The equations and appropriate conditions for them are presented in the Appendix. We obtain the second-order approximations of dopant concentrations on all parameters ε_L, ξ. The approximation could be used for all parameters within the following intervals $0\leq \varepsilon_L \sim 0.2$, $0\leq \xi \sim 0.2$.

Analysis of spatiotemporal distributions of dopant concentrations has been done analytically by using the second-order approximation of dopant and radiation defects concentration. Farther the distribution has been amended numerically.

3. DISCUSSION

The relations, obtained in the previous section, give us possibility to analyze and compare redistribution of dopant and radiation defects in homogenous sample and heterostructure in Fig. 1 during annealing. Spatial distributions in materials with OL and without OL are presented in Fig.2 for different values of annealing time. Curves 1, 2 and 3 correspond to distributions of concentration of dopant in homogenous sample without OL after annealing of radiation defects. Curves 4, 5 and 6 correspond to distributions of concentration of dopant in the both: initial sample and OL. We consider the distributions of concentration of dopant for such example, when thicknesses of both layers (initial sample and OL) are equal to each other.

The figure shows, that during annealing of radiation defects one could obtain spreading of dopant. We obtain, that presents of OL leads to increasing of difference between halfs of width at half height of the distributions. However the difference could be obtained, when value of dopant diffusion coefficient in OL outstrips value of dopant diffusion coefficient in initial homogenous sample. Due to the difference one can obtain shifting of *p*-*n*-junction in the direction of OL. Spatial distributions of radiation defects are qualitatively same with spatial distributions of dopant. One could be decrease quantity of radiation defects by using multistage ion implantation and annealing of radiation defects [10]. However in this situation one can obtain increasing of quantity of complexes of point defects [10]. It is known, that complexes of radiation defects are slow moving in comparison with point defects and atoms of dopant. In this situation increasing of difference between halfs of width at half height of distributions of concentrations of complexes of radiation defects distribution is behind from increasing of difference between halfs of width at half height of distributions of dopant concentration distribution. Hereby due to using OL one can obtain shifting of *p*-*n*-junction in area with smaller quantity of radiation defects.

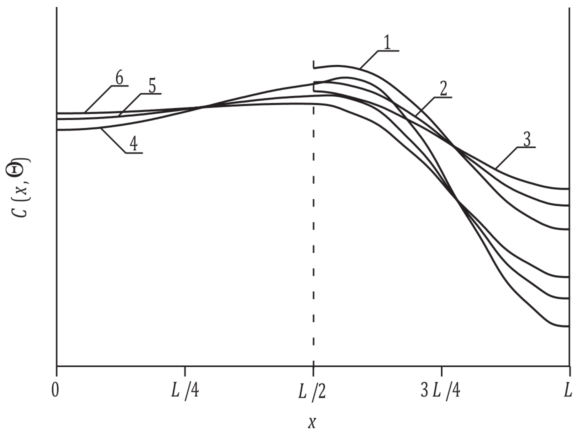

Fig. 2. Spatial distributions of dopant in homogenous sample (curves 1-3) and in heterostructure with overlayer (curves 4-6). Increasing of number of curves corresponds to increasing of annealing time

We analyzed spatial distributions of concentrations of point defects. The distributions are presented in Fig. 3. The figure shows, that quantity of radiation defects decreases in area of *p*-*n*-junction. Reason of the decreasing is smaller value of diffusion coefficient of point radiation defects in comparison with value of dopant diffusion coefficient [2].

4. CONCLUSION

In this paper we consider redistributions of dopant and radiation defects in an implanted-junction rectifier in the system homogenous sample – overlayer during annealing of radiation defects. Recommendations to decrease quantity of radiation defects in the implanted-junction rectifier have been formulated.

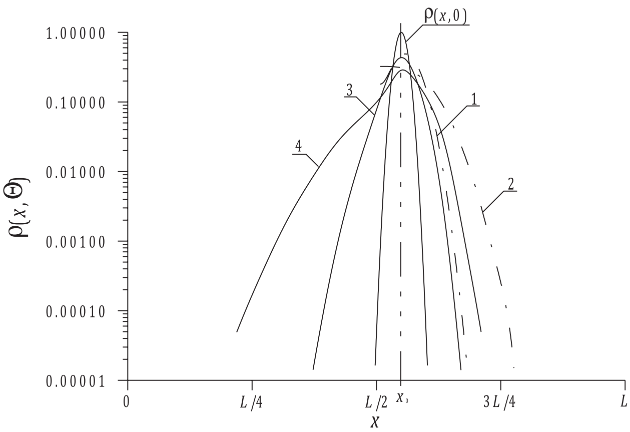

Fig. 3. Spatial distributions of point radiation defects in homogenous sample (curves 1 and 2) and in heterostructure with overlayer (curves 3 and 4). Increasing of number of curves corresponds to increasing of annealing time

Appendix

Equations for functions $\tilde{I}_{ijk}(\chi,\vartheta)$ and $\tilde{V}_{ijk}(\chi,\vartheta)$ ($i \geq 0$, $j \geq 0$, $k \geq 0$) could be written as

$$\frac{\partial \tilde{I}_{000}(\chi,\vartheta)}{\partial \vartheta}=\sqrt{\frac{D_{0I}}{D_{0V}}}\frac{\partial^2 \tilde{I}_{000}(\chi,\vartheta)}{\partial \chi^2},\quad \frac{\partial \tilde{V}_{000}(\chi,\vartheta)}{\partial \vartheta}=\sqrt{\frac{D_{0V}}{D_{0I}}}\frac{\partial^2 \tilde{V}_{000}(\chi,\vartheta)}{\partial \chi^2};$$

$$\begin{cases}\dfrac{\partial \tilde{I}_{i00}(\chi,\vartheta)}{\partial \vartheta}=\sqrt{\dfrac{D_{0I}}{D_{0V}}}\dfrac{\partial^2 \tilde{I}_{i00}(\chi,\vartheta)}{\partial \chi^2}+\sqrt{\dfrac{D_{0I}}{D_{0V}}}\dfrac{\partial}{\partial \chi}\left[g_I(\chi,T)\dfrac{\partial \tilde{I}_{i-100}(\chi,\vartheta)}{\partial \chi}\right]\\ \dfrac{\partial \tilde{V}_{i00}(\chi,\vartheta)}{\partial \vartheta}=\sqrt{\dfrac{D_{0V}}{D_{0I}}}\dfrac{\partial^2 \tilde{V}_{i00}(\chi,\vartheta)}{\partial \chi^2}+\sqrt{\dfrac{D_{0V}}{D_{0I}}}\dfrac{\partial}{\partial \chi}\left[g_V(\chi,T)\dfrac{\partial \tilde{V}_{i-100}(\chi,\vartheta)}{\partial \chi}\right]\end{cases},\ i \geq 1;$$

$$\begin{cases}\dfrac{\partial \tilde{I}_{010}(\chi,\vartheta)}{\partial \vartheta}=\sqrt{\dfrac{D_{0I}}{D_{0V}}}\dfrac{\partial^2 \tilde{I}_{010}(\chi,\vartheta)}{\partial \chi^2}-\left[1+\varepsilon_{I,V}g_{I,V}(\chi,T)\right]\tilde{I}_{000}(\chi,\vartheta)\tilde{V}_{000}(\chi,\vartheta)\\ \dfrac{\partial \tilde{V}_{010}(\chi,\vartheta)}{\partial \vartheta}=\sqrt{\dfrac{D_{0V}}{D_{0I}}}\dfrac{\partial^2 \tilde{V}_{010}(\chi,\vartheta)}{\partial \chi^2}-\left[1+\varepsilon_{I,V}g_{I,V}(\chi,T)\right]\tilde{I}_{000}(\chi,\vartheta)\tilde{V}_{000}(\chi,\vartheta)\end{cases};$$

$$\begin{cases} \dfrac{\partial \tilde{I}_{020}(\chi,\vartheta)}{\partial \vartheta} = \sqrt{\dfrac{D_{0I}}{D_{0V}}}\dfrac{\partial^2 \tilde{I}_{020}(\chi,\vartheta)}{\partial \chi^2} - \\ \qquad -\left[1+\varepsilon_{I,V} g_{I,V}(\chi,T)\right]\left[\tilde{I}_{010}(\chi,\vartheta)\tilde{V}_{000}(\chi,\vartheta)+\tilde{I}_{000}(\chi,\vartheta)\tilde{V}_{010}(\chi,\vartheta)\right] \\ \dfrac{\partial \tilde{V}_{020}(\chi,\vartheta)}{\partial \vartheta} = \sqrt{\dfrac{D_{0I}}{D_{0V}}}\dfrac{\partial^2 \tilde{V}_{020}(\chi,\vartheta)}{\partial \chi^2} - \\ \qquad -\left[1+\varepsilon_{I,V} g_{I,V}(\chi,T)\right]\left[\tilde{I}_{010}(\chi,\vartheta)\tilde{V}_{000}(\chi,\vartheta)+\tilde{I}_{000}(\chi,\vartheta)\tilde{V}_{010}(\chi,\vartheta)\right] \end{cases};$$

$$\begin{cases} \dfrac{\partial \tilde{I}_{001}(\chi,\vartheta)}{\partial \vartheta} = \sqrt{\dfrac{D_{0I}}{D_{0V}}}\dfrac{\partial^2 \tilde{I}_{001}(\chi,\vartheta)}{\partial \chi^2} - \left[1+\varepsilon_{I,I} g_{I,I}(\chi,T)\right]\tilde{I}_{000}^2(\chi,\vartheta) \\ \dfrac{\partial \tilde{V}_{001}(\chi,\vartheta)}{\partial \vartheta} = \sqrt{\dfrac{D_{0V}}{D_{0I}}}\dfrac{\partial^2 \tilde{V}_{001}(\chi,\vartheta)}{\partial \chi^2} - \left[1+\varepsilon_{I,I} g_{I,I}(\chi,T)\right]\tilde{V}_{000}^2(\chi,\vartheta) \end{cases};$$

$$\begin{cases} \dfrac{\partial \tilde{I}_{110}(\chi,\vartheta)}{\partial \vartheta} = \sqrt{\dfrac{D_{0I}}{D_{0V}}}\dfrac{\partial^2 \tilde{I}_{110}(\chi,\vartheta)}{\partial \chi^2} + \sqrt{\dfrac{D_{0I}}{D_{0V}}}\dfrac{\partial}{\partial \chi}\left[g_I(\chi,T)\dfrac{\partial \tilde{I}_{010}(\chi,\vartheta)}{\partial \chi}\right] - \\ \qquad -\left[1+\varepsilon_{I,I} g_{I,I}(\chi,T)\right]\left[\tilde{I}_{100}(\chi,\vartheta)\tilde{V}_{000}(\chi,\vartheta)+\tilde{I}_{000}(\chi,\vartheta)\tilde{V}_{100}(\chi,\vartheta)\right] \\ \dfrac{\partial \tilde{V}_{110}(\chi,\vartheta)}{\partial \vartheta} = \sqrt{\dfrac{D_{0V}}{D_{0I}}}\dfrac{\partial^2 \tilde{V}_{110}(\chi,\vartheta)}{\partial \chi^2} + \sqrt{\dfrac{D_{0V}}{D_{0I}}}\dfrac{\partial}{\partial \chi}\left[g_V(\chi,T)\dfrac{\partial \tilde{V}_{010}(\chi,\vartheta)}{\partial \chi}\right] - \\ \qquad -\left[1+\varepsilon_{V,V} g_{V,V}(\chi,T)\right]\left[\tilde{V}_{100}(\chi,\vartheta)\tilde{I}_{000}(\chi,\vartheta)+\tilde{V}_{000}(\chi,\vartheta)\tilde{I}_{100}(\chi,\vartheta)\right] \end{cases};$$

$$\begin{cases} \dfrac{\partial \tilde{I}_{002}(\chi,\vartheta)}{\partial \vartheta} = \sqrt{\dfrac{D_{0I}}{D_{0V}}}\dfrac{\partial^2 \tilde{I}_{002}(\chi,\vartheta)}{\partial \chi^2} - \left[1+\varepsilon_{I,I} g_{I,I}(\chi,T)\right]\tilde{I}_{001}(\chi,\vartheta)\tilde{I}_{000}(\chi,\vartheta) \\ \dfrac{\partial \tilde{V}_{002}(\chi,\vartheta)}{\partial \vartheta} = \sqrt{\dfrac{D_{0V}}{D_{0I}}}\dfrac{\partial^2 \tilde{V}_{002}(\chi,\vartheta)}{\partial \chi^2} - \left[1+\varepsilon_{I,I} g_{I,I}(\chi,T)\right]\tilde{V}_{001}(\chi,\vartheta)\tilde{V}_{000}(\chi,\vartheta) \end{cases};$$

$$\begin{cases} \dfrac{\partial \tilde{I}_{101}(\chi,\vartheta)}{\partial \vartheta} = \sqrt{\dfrac{D_{0I}}{D_{0V}}}\dfrac{\partial^2 \tilde{I}_{101}(\chi,\vartheta)}{\partial \chi^2} + \sqrt{\dfrac{D_{0I}}{D_{0V}}}\dfrac{\partial}{\partial \chi}\left[g_I(\chi,T)\dfrac{\partial \tilde{I}_{001}(\chi,\vartheta)}{\partial \chi}\right] - \\ \qquad -\left[1+\varepsilon_I g_I(\chi,T)\right]\tilde{I}_{100}(\chi,\vartheta)\tilde{V}_{000}(\chi,\vartheta) \\ \dfrac{\partial \tilde{V}_{101}(\chi,\vartheta)}{\partial \vartheta} = \sqrt{\dfrac{D_{0V}}{D_{0I}}}\dfrac{\partial^2 \tilde{V}_{101}(\chi,\vartheta)}{\partial \chi^2} + \sqrt{\dfrac{D_{0V}}{D_{0I}}}\dfrac{\partial}{\partial \chi}\left[g_V(\chi,T)\dfrac{\partial \tilde{V}_{001}(\chi,\vartheta)}{\partial \chi}\right] - \\ \qquad -\left[1+\varepsilon_V g_V(\chi,T)\right]\tilde{I}_{000}(\chi,\vartheta)\tilde{V}_{100}(\chi,\vartheta) \end{cases};$$

$$\begin{cases}\dfrac{\partial \tilde{I}_{011}(\chi,\vartheta)}{\partial \vartheta}=\sqrt{\dfrac{D_{0I}}{D_{0V}}}\dfrac{\partial^2 \tilde{I}_{011}(\chi,\vartheta)}{\partial \chi^2}-\left[1+\varepsilon_{I,I}g_{I,I}(\chi,T)\right]\tilde{I}_{000}(\chi,\vartheta)\tilde{I}_{010}(\chi,\vartheta)-\\ \qquad -\left[1+\varepsilon_{I,V}g_{I,V}(\chi,T)\right]\tilde{I}_{001}(\chi,\vartheta)\tilde{V}_{000}(\chi,\vartheta)\\ \dfrac{\partial \tilde{V}_{011}(\chi,\vartheta)}{\partial \vartheta}=\sqrt{\dfrac{D_{0V}}{D_{0I}}}\dfrac{\partial^2 \tilde{V}_{011}(\chi,\vartheta)}{\partial \chi^2}-\left[1+\varepsilon_{V,V}g_{V,V}(\chi,T)\right]\tilde{V}_{000}(\chi,\vartheta)\tilde{V}_{010}(\chi,\vartheta)-\\ \qquad -\left[1+\varepsilon_{I,V}g_{I,V}(\chi,T)\right]\tilde{I}_{000}(\chi,\vartheta)\tilde{V}_{001}(\chi,\vartheta)\end{cases};$$

Conditions for the functions $\tilde{I}_{ijk}(\chi,\vartheta)$ and $\tilde{V}_{ijk}(\chi,\vartheta)$ ($i \geq 0$, $j \geq 0$, $k \geq 0$) are

$$\tilde{\rho}_{000}(\chi,0)=f_\rho(\chi)/\rho^*,\ \tilde{\rho}_{ijk}(\chi,0)=0 \text{ (i ≥1, j ≥1, k ≥1)};$$

$$\left.\frac{\partial \tilde{\rho}_{ijk}(\chi,\vartheta)}{\partial \chi}\right|_{x=0}=\left.\frac{\partial \tilde{\rho}_{ijk}(\chi,\vartheta)}{\partial \chi}\right|_{x=1}=0, \text{ (i ≥0, j ≥0, k ≥0)}.$$

Solutions of these equations could be written in the following form

$$\tilde{\rho}_{000}(\chi,\vartheta)=\frac{1}{L}+\frac{2}{L}\sum_{n=1}^{\infty}F_{n\rho}c(\chi)e_{n\rho}(\vartheta),$$

where $e_{nI}(\vartheta)=\exp\left(-\pi^2n^2\vartheta\sqrt{D_{0V}/D_{0I}}\right)$, $e_{nV}(\vartheta)=\exp\left(-\pi^2n^2\vartheta\sqrt{D_{0I}/D_{0V}}\right)$, $c_n(\chi) = cos\ (\pi\ \nu\ \chi)$,
$F_{n\rho}=\frac{1}{\rho^*}\int_0^1\cos(\pi n u)f_{n\rho}(u)du$;

$$\begin{cases}\tilde{I}_{i00}(\chi,\vartheta)=-2\pi\sqrt{\dfrac{D_{0I}}{D_{0V}}}\sum_{n=1}^{\infty}nc_n(\chi)e_{nI}(\vartheta)\int_0^{\vartheta}e_{nI}(-\tau)\int_0^1 s_n(u)g_I(u,T)\dfrac{\partial \tilde{I}_{i-100}(u,\tau)}{\partial u}du\,d\tau\\ \tilde{V}_{i00}(\chi,\vartheta)=-2\pi\sqrt{\dfrac{D_{0V}}{D_{0I}}}\sum_{n=1}^{\infty}nc_n(\chi)e_{nV}(\vartheta)\int_0^{\vartheta}e_{nV}(-\tau)\int_0^1 s_n(u)g_V(u,T)\dfrac{\partial \tilde{V}_{i-100}(u,\tau)}{\partial u}du\,d\tau\end{cases}, i \geq 1,$$

where $\sigma_n(\chi) = sin\ (\pi\ n\ \chi)$;

$$\tilde{\rho}_{010}(\chi,\vartheta)=-2\sum_{n=1}^{\infty}c_n(\chi,\varphi)e_{n\rho}(\vartheta)\int_0^{\vartheta}e_{n\rho}(-\tau)\int_0^1 c(u)\left[1+\varepsilon_{I,V}g_{I,V}(u,T)\right]\tilde{I}_{000}(u,\tau)\tilde{V}_{000}(u,\tau)du\,d\tau;$$

$$\tilde{\rho}_{020}(\chi,\vartheta)=-2\sqrt{\frac{D_{0I}}{D_{0V}}}\sum_{n=1}^{\infty}c_n(\chi)e_{n\rho}(\vartheta)\int_0^{\vartheta}e_{n\rho}(-\tau)\int_0^1 c(u)\left[1+\varepsilon_{I,V}g_{I,V}(u,T)\right]\times;$$

$$\times\left[\tilde{I}_{010}(\chi,\vartheta)\tilde{V}_{000}(\chi,\vartheta)+\tilde{I}_{000}(\chi,\vartheta)\tilde{V}_{010}(\chi,\vartheta)\right]du\,d\tau;$$

$$\begin{cases} \tilde{I}_{110}(\chi,\vartheta)=-2\pi\sqrt{\frac{D_{0I}}{D_{0V}}}\sum_{n=1}^{\infty} n\,c_n(\chi)e_{nI}(\vartheta)\int_0^{\vartheta} e_{nI}(-\tau)\int_0^1 s_n(u)g_I(u,T)\frac{\partial \tilde{I}_{010}(u,\tau)}{\partial u}\,d\,u\,d\,\tau- \\ -2\sum_{n=1}^{\infty} c_n(\chi)e_{nI}(\vartheta)\int_0^{\vartheta} e_{nI}(-\tau)\int_0^1 c_n(u)\left[\tilde{I}_{100}(u,\tau)\tilde{V}_{000}(u,\tau)+\tilde{I}_{000}(u,\tau)\tilde{V}_{100}(u,\tau)\right]\times \\ \times\left[1+\varepsilon_{I,V}g_{I,V}(u,T)\right]d\,u\,d\,\tau \\ \tilde{V}_{110}(\chi,\vartheta)=-2\pi\sqrt{\frac{D_{0V}}{D_{0I}}}\sum_{n=1}^{\infty} n\,c_n(\chi)e_{nV}(\vartheta)\int_0^{\vartheta} e_{nV}(-\tau)\int_0^1 s_n(u)g_V(u,T)\frac{\partial \tilde{V}_{010}(u,\tau)}{\partial u}\,d\,u\,d\,\tau- \\ -2\sum_{n=1}^{\infty} c_n(\chi)e_{nV}(\vartheta)\int_0^{\vartheta} e_{nV}(-\tau)\int_0^1 c_n(u)\left[\tilde{I}_{000}(u,\tau)\tilde{V}_{100}(u,\tau)+\tilde{I}_{100}(u,\tau)\tilde{V}_{000}(u,\tau)\right]\times \\ \times\left[1+\varepsilon_{I,V}g_{I,V}(u,T)\right]d\,u\,d\,\tau \end{cases};$$

$$\tilde{\rho}_{001}(\chi,\vartheta)=-2\sum_{n=1}^{\infty} c_n(\chi)e_{n\rho}(\vartheta)\int_0^{\vartheta} e_{n\rho}(-\tau)\int_0^1 c_n(u)\left[1+\varepsilon_{\rho,\rho}g_{\rho,\rho}(u,T)\right]\tilde{\rho}_{000}^2(u,\tau)\,d\,u\,d\,\tau;$$

$$\tilde{\rho}_{002}(\chi,\vartheta)=-2\sum_{n=1}^{\infty} c_n(\chi)e_{n\rho}(\vartheta)\int_0^{\vartheta} e_{n\rho}(-\tau)\int_0^1 c_n(u)\left[1+\varepsilon_{\rho,\rho}g_{\rho,\rho}(u,T)\right]\tilde{\rho}_{001}(u,\tau)\tilde{\rho}_{000}(u,\tau)\,d\,u\,d\,\tau;$$

$$\begin{cases} \tilde{I}_{101}(\chi,\vartheta)=-2\pi\sqrt{\frac{D_{0I}}{D_{0V}}}\sum_{n=1}^{\infty} n\,c_n(\chi)e_{nI}(\vartheta)\int_0^{\vartheta} e_{nI}(-\tau)\int_0^1 s_n(u)g_I(u,T)\frac{\partial \tilde{I}_{001}(u,\tau)}{\partial u}\,d\,u\,d\,\tau- \\ \quad -2\sum_{n=1}^{\infty} c_n(\chi)e_{nI}(\vartheta)\int_0^{\vartheta} e_{nI}(-\tau)\int_0^1 c_n(u)\left[1+\varepsilon_{I,V}g_{I,V}(u,T)\right]\tilde{I}_{100}(u,\tau)\tilde{V}_{000}(u,\tau)\,d\,u\,d\,\tau \\ \tilde{V}_{101}(\chi,\vartheta)=-2\pi\sqrt{\frac{D_{0V}}{D_{0I}}}\sum_{n=1}^{\infty} n\,c_n(\chi)e_{nV}(\vartheta)\int_0^{\vartheta} e_{nV}(-\tau)\int_0^1 s_n(u)g_V(u,T)\frac{\partial \tilde{V}_{001}(u,\tau)}{\partial u}\,d\,u\,d\,\tau- \\ \quad -2\sum_{n=1}^{\infty} c_n(\chi)e_{nV}(\vartheta)\int_0^{\vartheta} e_{nV}(-\tau)\int_0^1 c_n(u)\left[1+\varepsilon_{I,V}g_{I,V}(u,T)\right]\tilde{I}_{000}(u,\tau)\tilde{V}_{100}(u,\tau)\,d\,u\,d\,\tau \end{cases};$$

$$\begin{cases} \tilde{I}_{011}(\chi,\vartheta)=-2\sum_{n=1}^{\infty} c_n(\chi)e_{nI}(\vartheta)\int_0^{\vartheta} e_{nI}(-\tau)\int_0^1 c_n(u)\left\{\left[1+\varepsilon_{I,I}g_{I,I}(u,T)\right]\tilde{I}_{000}(u,\tau)\tilde{I}_{010}(u,\tau)+\right. \\ \qquad \left.+\left[1+\varepsilon_{I,V}g_{I,V}(u,T)\right]\tilde{I}_{001}(u,\tau)\tilde{V}_{000}(u,\tau)\right\}d\,u\,d\,\tau \\ \tilde{V}_{011}(\chi,\vartheta)=-2\sum_{n=1}^{\infty} c_n(\chi)e_{nV}(\vartheta)\int_0^{\vartheta} e_{nV}(-\tau)\int_0^1 c_n(u)\left\{\left[1+\varepsilon_{V,V}g_{V,V}(u,T)\right]\tilde{V}_{000}(u,\tau)\tilde{V}_{010}(u,\tau)+\right. \\ \qquad \left.+\left[1+\varepsilon_{I,V}g_{I,V}(u,T)\right]\tilde{I}_{001}(u,\tau)\tilde{V}_{000}(u,\tau)\right\}d\,u\,d\,\tau. \end{cases}$$

Equations for the functions $\Phi_{\rho i}(x,t)$ ($i \geq 0$), boundary and initial conditions for them could be written as

$$\begin{cases} \frac{\partial \Phi_{I0}(x,t)}{\partial t}=D_{0\Phi I}\frac{\partial^2 \Phi_{I0}(x,t)}{\partial x^2}+k_{I,I}(x,T)I^2(x,t)-k_I(x,T)I(x,t) \\ \frac{\partial \Phi_{V0}(x,t)}{\partial t}=D_{0\Phi V}\frac{\partial^2 \Phi_{V0}(x,t)}{\partial x^2}+k_{V,V}(x,T)V^2(x,t)-k_V(x,T)V(x,t) \end{cases};$$

$$\begin{cases} \dfrac{\partial \Phi_{I\,i}(x,t)}{\partial t} = D_{0\Phi I}\dfrac{\partial^2 \Phi_{I\,i}(x,t)}{\partial x^2} + D_{0\Phi I}\dfrac{\partial}{\partial x}\left[g_{\Phi I}(x,T)\dfrac{\partial \Phi_{I\,i-1}(x,t)}{\partial x}\right] \\ \dfrac{\partial \Phi_{V\,i}(x,t)}{\partial t} = D_{0\Phi V}\dfrac{\partial^2 \Phi_{V\,i}(x,t)}{\partial x^2} + D_{0\Phi V}\dfrac{\partial}{\partial x}\left[g_{\Phi V}(x,T)\dfrac{\partial \Phi_{V\,i-1}(x,t)}{\partial x}\right] \end{cases}, \; i\geq 1;$$

$$\left.\frac{\partial \Phi_{\rho\,i}(x,t)}{\partial x}\right|_{x=0} = \left.\frac{\partial \Phi_{\rho\,i}(x,t)}{\partial x}\right|_{x=L} = 0, \; i\geq 0;\; F_{r0}(x,0)=f_{Fr}(x),\; F_{ri}(x,0)=0,\; i\geq 1.$$

Solutions for the equations are

$$\Phi_{\rho 0}(x,t) = \frac{1}{L} + \frac{2}{L}\sum_{n=1}^{\infty} F_{n\Phi_\rho}\, c(x)\, e_{n\Phi_\rho}(t)\cdot$$

Here $e_{n\Phi_\rho}(t) = \exp\left(-\pi^2 n^2 D_{0\Phi_\rho} t / L^2\right)$, $F_{n\Phi_\rho} = \int_0^L c_n(u) f_{\Phi_\rho}(u)\, du$, $c_n(L) = cos\ (\pi\ n\ x/L)$;

$$\Phi_{\rho\,i}(x,t) = -\frac{2\pi}{L^2}\sum_{n=1}^{\infty} n\, c_n(x) e_{\Phi_\rho n}(t)\int_0^t e_{\Phi_\rho n}(-\tau)\int_0^L s_n(u) g_{\Phi_\rho}(u,T)\frac{\partial \Phi_{I_\rho i-1}(u,\tau)}{\partial u}\, du\, d\tau, \; \mathrm{i}\geq 1.$$

Here $s_n(L) = sin\ (\pi\ n\ x/L)$.

Equations for the functions $C_{ij}(x,t)$ ($i \geq 0$, $j \geq 0$), boundary and initial conditions could be written as

$$\frac{\partial C_{00}(x,t)}{\partial t} = D_{0L}\frac{\partial^2 C_{00}(x,t)}{\partial x^2};$$

$$\frac{\partial C_{i0}(x,t)}{\partial t} = D_{0L}\frac{\partial^2 C_{i0}(x,t)}{\partial x^2} + D_{0L}\frac{\partial}{\partial x}\left[g_L(x,T)\frac{\partial C_{i-10}(x,t)}{\partial x}\right], \; \mathrm{i}\geq 1;$$

$$\frac{\partial C_{01}(x,t)}{\partial t} = D_{0L}\frac{\partial^2 C_{01}(x,t)}{\partial x^2} + D_{0L}\frac{\partial}{\partial x}\left[\frac{C_{00}^{\gamma}(x,t)}{P^{\gamma}(x,T)}\frac{\partial C_{00}(x,t)}{\partial x}\right];$$

$$\frac{\partial C_{02}(x,t)}{\partial t} = D_{0L}\frac{\partial^2 C_{02}(x,t)}{\partial x^2} + D_{0L}\frac{\partial}{\partial x}\left[\frac{C_{00}^{\gamma}(x,t)}{P^{\gamma}(x,T)}\frac{\partial C_{01}(x,t)}{\partial x}\right] + D_{0L}\frac{\partial}{\partial x}\left[C_{01}(x,t)\frac{C_{00}^{\gamma-1}(x,t)}{P^{\gamma}(x,T)}\frac{\partial C_{00}(x,t)}{\partial x}\right];$$

$$\frac{\partial C_{11}(x,t)}{\partial t} = D_{0L}\frac{\partial^2 C_{11}(x,t)}{\partial x^2} + D_{0L}\frac{\partial}{\partial x}\left[C_{10}(x,t)\frac{C_{00}^{\gamma-1}(x,t)}{P^{\gamma}(x,T)}\frac{\partial C_{00}(x,t)}{\partial x}\right] + D_{0L}\frac{\partial}{\partial x}\left[\frac{C_{00}^{\gamma}(x,t)}{P^{\gamma}(x,T)}\frac{\partial C_{10}(x,t)}{\partial x}\right] + \frac{\partial}{\partial x}\left[g_L(x,T)\frac{\partial C_{01}(x,t)}{\partial x}\right];$$

$$\left.\frac{\partial C_{ij}(x,t)}{\partial x}\right|_{x=0}=\left.\frac{\partial C_{ij}(x,t)}{\partial x}\right|_{x=L}=0,\ i\geq 0,\ j\geq 0;\ C_{00}(x,0)=f_C(x),\ C_{ij}(x,0)=0,\ i\geq 1,\ j\geq 1.$$

$$C_{00}(x,t)=\frac{1}{L}+\frac{2}{L}\sum_{n=1}^{\infty}F_{nC}c(x)e_{nC}(t).$$

Here $e_{nC}(t)=\exp\left(-\pi^2 n^2 D_{0C}t/L^2\right)$, $F_{nC}=\int_0^L c_n(u)f_C(u)\,du$;

$$C_{i0}(x,t)=-\frac{2\pi}{L^2}\sum_{n=1}^{\infty}nF_{nC}c_n(x)e_{nC}(t)\int_0^t e_{nC}(-\tau)\int_0^L s_n(u)g_L(u,T)\frac{\partial C_{i-10}(u,\tau)}{\partial u}\,du\,d\tau,\ \mathrm{i}\geq 1;$$

$$C_{01}(x,t)=-\frac{2\pi}{L^2}\sum_{n=1}^{\infty}nF_{nC}c_n(x)e_{nC}(t)\int_0^t e_{nC}(-\tau)\int_0^L s_n(u)\frac{C_{00}^{\gamma}(u,\tau)}{P^{\gamma}(u,T)}\frac{\partial C_{00}(u,\tau)}{\partial u}\,du\,d\tau;$$

$$C_{02}(x,t)=-\frac{2\pi}{L^2}\sum_{n=1}^{\infty}nF_{nC}c_n(x)e_{nC}(t)\int_0^t e_{nC}(-\tau)\int_0^L s_n(u)C_{01}(u,\tau)\frac{C_{00}^{\gamma-1}(u,\tau)}{P^{\gamma}(u,T)}\frac{\partial C_{00}(u,\tau)}{\partial u}\,du\,d\tau-$$

$$-\frac{2\pi}{L^2}\sum_{n=1}^{\infty}nF_{nC}c_n(x)e_{nC}(t)\int_0^t e_{nC}(-\tau)\int_0^L s_n(u)\frac{C_{00}^{\gamma}(u,\tau)}{P^{\gamma}(u,T)}\frac{\partial C_{01}(u,\tau)}{\partial u}\,du\,d\tau$$

$$C_{11}(x,t)=-\frac{2\pi}{L^2}\sum_{n=1}^{\infty}nF_{nC}c_n(x)e_{nC}(t)\int_0^t e_{nC}(-\tau)\int_0^L s_n(u)g_L(u,T)\frac{\partial C_{01}(u,\tau)}{\partial u}\,du\,d\tau-\frac{2\pi}{L^2}\sum_{n=1}^{\infty}F_{nC}\times$$

$$\times n\,c_n(x)e_{nC}(t)\int_0^t e_{nC}(-\tau)\int_0^L s_n(u)\frac{C_{00}^{\gamma}(u,\tau)}{P^{\gamma}(u,T)}\frac{\partial C_{10}(u,\tau)}{\partial u}\,du\,d\tau-\frac{2\pi}{L^2}\sum_{n=1}^{\infty}n\,c_n(x)e_{nC}(t)\int_0^t e_{nC}(-\tau)\times$$

$$\times F_{nC}\int_0^L s_n(u)C_{10}(u,\tau)\frac{C_{00}^{\gamma-1}(u,\tau)}{P^{\gamma}(u,T)}\frac{\partial C_{00}(u,\tau)}{\partial u}\,du\,d\tau.$$

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