

AN APPROACH FOR OPTIMIZATION OF MANUFACTURE MULTIEmitter HETEROTRANSISTORS

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ABSTRACT

In this paper we introduced an approach to model manufacture process of a multiemitter heterotransistor. The approach gives us also possibility to optimize manufacture process. p-n-junctions, which include into the multiemitter heterotransistor, have higher sharpness and higher homogeneity of dopants distributions in enriched by the dopant area.

KEYWORDS

Multiemitter heterotransistor, Approach to optimize technological processes.

1. INTRODUCTION

Logical elements often include into itself multiemitter transistors [1-4]. To manufacture bipolar transistors it could be used dopant diffusion, ion doping or epitaxial layer [1-8]. It is attracted an interest increasing of sharpness of p-n-junctions, which include into bipolar transistors and decreasing of dimensions of the transistors, which include into integrated circuits [1-4]. Dimensions of transistors will be decreased by using inhomogenous distribution of temperature during laser or microwave types of annealing [9,10], using defects of materials (for example, defects could be generated during radiation processing of materials) [11-14], native inhomogeneity (multilayer property) of heterostructure [12-14].

Framework this paper we consider a heterostructure, which consist of a substrate and three epitaxial layers (see Fig. 1). Some dopants are infused in the epitaxial layers to manufacture p and n types of conductivities during manufacture a multiemitter transistor. Let us consider two cases: infusion of dopant by diffusion or ion implantation. Farther in the first case we consider annealing of dopant so long, that after the annealing the dopants should achieve interfaces between epitaxial layers. In this case one can obtain increasing of sharpness of p-n-junctions [12-14]. The increasing of sharpness could be obtained under conditions, when values of dopant diffusion coefficients in last epitaxial layers is larger, than values of dopant diffusion coefficient in average epitaxial layer. At the same time homogeneity of dopant distributions in doped areas increases. It is attracted an interest higher doping of last epitaxial layers, than doping of average epitaxial layer, because the higher doping gives us possibility to increase sharpness of p-n-junctions. It is

also practicable to choose materials of epitaxial layers and substrate so; those values of dopant diffusion coefficients in the substrate should be smaller, than in the epitaxial layer. In this situation one can obtain thinner transistor. In the case of ion doping of heterostructure it should be done annealing of radiation defects. It is practicable to choose so regimes of annealing of radiation defects, that dopant should achieves interface between epitaxial layers. At the same time the dopant could not diffuse into another epitaxial layer. If dopant did not achieves interface between epitaxial layers during annealing of radiation defects, additional annealing of dopant required.

Main aims of the present paper are analysis of dynamics of redistribution of dopants in considered heterostructure (Figs. 1) and optimization of annealing times of dopants. In some recent papers analogous analysis have been done [4,10,12-14]. However we can not find in literature any similar heterostructures as we consider in the paper.

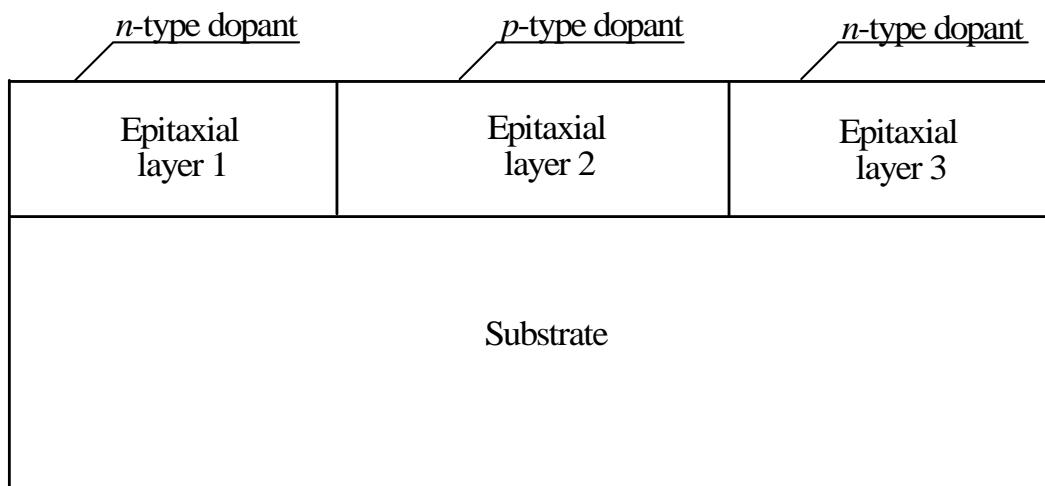


Fig. 1a. Heterostructure, which consist of a substrate and three epitaxial layers. View from above

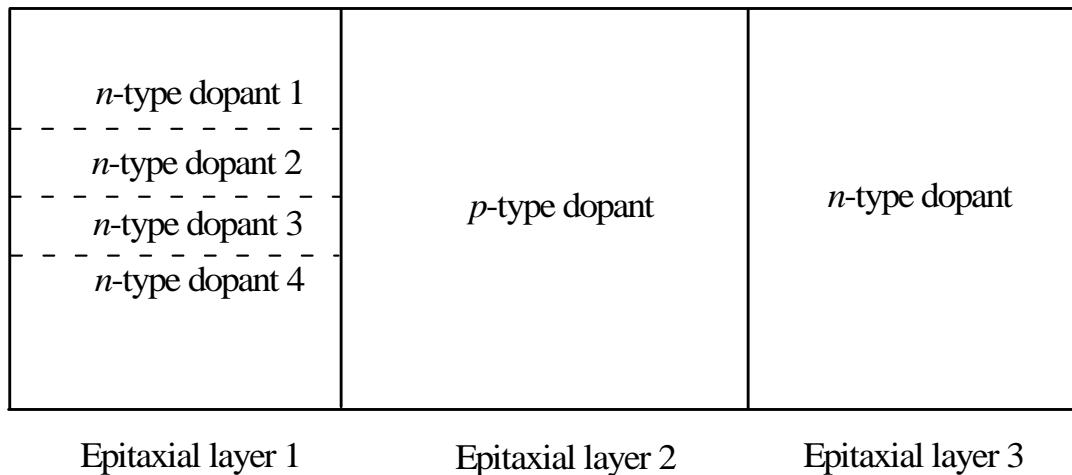


Fig. 1b. Heterostructure, which consist of a substrate and three epitaxial layers. View from one side

2. Method of Analysis

Redistribution of dopant in the considered heterostructure has been described by the second Fick's law [1-4]

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

with boundary and initial conditions

$$\begin{aligned} \left. \frac{\partial C(x, y, z, t)}{\partial x} \right|_{x=0} &= 0, \quad \left. \frac{\partial C(x, y, z, t)}{\partial x} \right|_{x=L_x} = 0, \quad \left. \frac{\partial C(x, y, z, t)}{\partial y} \right|_{y=0} = 0, \quad \left. \frac{\partial C(x, y, z, t)}{\partial y} \right|_{y=L_y} = 0, \\ \left. \frac{\partial C(x, y, z, t)}{\partial z} \right|_{z=0} &= 0, \quad \left. \frac{\partial C(x, y, z, t)}{\partial z} \right|_{z=L_z} = 0, \quad C(x, y, z, 0) = f_C(x, y, z). \end{aligned} \quad (2)$$

Here $C(x, y, z, t)$ is the spatio-temporal distribution of concentration of dopant; x, y, z and t are current coordinates and times; D_c is the dopant diffusion coefficient. Value of dopant diffusion coefficient depends on properties of materials in layers of heterostructure, speed of heating and cooling of heterostructure (with account Arrhenius low), spatio-temporal distributions of concentrations of dopants and radiation defects. Two last dependences of dopant diffusion coefficient could be approximated by the following relation [15,16]

$$D_c = D_L(x, y, z, T) \left[1 + \xi \frac{C^\gamma(x, y, z, t)}{P^\gamma(x, y, z, T)} \right] \left[1 + \zeta_1 \frac{V(x, y, z, t)}{V^*} + \zeta_2 \frac{V^2(x, y, z, t)}{(V^*)^2} \right]. \quad (3)$$

Here $D_L(x, y, z, T)$ is the spatial (due to inhomogeneity () of heterostructure) and temperature (due to Arrhenius low) dependences of dopant diffusion coefficient; $P(x, y, z, T)$ is the limit of solubility of dopant; parameter γ depends of properties of materials and could be integer in the interval $\gamma \in [1, 3]$ [15]; $V(x, y, z, t)$ is the spatio-temporal distribution of concentration of radiation vacancies; V^* is the equilibrium distribution of vacancies. Concentrational dependence of dopant diffusion coefficient has been discussed in details in [15]. It should be noted, that radiation damage absents in the case of diffusion doping of heterostructure. In this situation $\zeta_1 = \zeta_2 = 0$. Spatio-temporal distributions of concentrations of point radiation defects could be determine by solution of the following system of equations [17-19]

$$\begin{aligned} \frac{\partial I(x, y, z, t)}{\partial t} &= \frac{\partial}{\partial x} \left[D_i(x, y, z, T) \frac{\partial I(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[D_i(x, y, z, T) \frac{\partial I(x, y, z, t)}{\partial y} \right] - I^2(x, y, z, t) \times \\ &\quad \times k_{i,i}(x, y, z, T) + \frac{\partial}{\partial z} \left[D_i(x, y, z, T) \frac{\partial I(x, y, z, t)}{\partial z} \right] - k_{i,v}(x, y, z, T) I(x, y, z, t) V(x, y, z, t) \end{aligned} \quad (4)$$

$$\begin{aligned} \frac{\partial V(x, y, z, t)}{\partial t} &= \frac{\partial}{\partial x} \left[D_v(x, y, z, T) \frac{\partial V(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[D_v(x, y, z, T) \frac{\partial V(x, y, z, t)}{\partial y} \right] - V^2(x, y, z, t) \times \\ &\quad \times k_{v,v}(x, y, z, T) + \frac{\partial}{\partial z} \left[D_v(x, y, z, T) \frac{\partial V(x, y, z, t)}{\partial z} \right] - k_{i,v}(x, y, z, T) I(x, y, z, t) V(x, y, z, t) \end{aligned}$$

with initial

$$\rho(x,y,z,0)=f_\rho(x,y,z) \quad (5a)$$

and boundary conditions

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

Here $\rho=I,V; I(x,y,z,t)$ is the spatio-temporal distribution of concentration of interstitials; $D_\rho(x,y,z,T)$ are diffusion coefficients of interstitials and vacancies; terms $V^2(x,y,z,t)$ and $I^2(x,y,z,t)$ correspond to generation of divacancies and analogous complexes of interstitials; $k_{I,V}(x,y,z,T)$, $k_{I,I}(x,y,z,T)$ and $k_{V,V}(x,y,z,T)$ parameters of recombination of point radiation defects and generation of complexes.

Spatio-temporal distributions of concentrations of divacancies $\Phi_V(x,y,z,t)$ and analogous complexes of interstitials $\Phi_I(x,y,z,t)$ will be determined by solving the following systems of equations [17-19]

$$\begin{aligned} \frac{\partial \Phi_I(x,y,z,t)}{\partial t} &= \frac{\partial}{\partial x} \left[D_{\phi_I}(x,y,z,T) \frac{\partial \Phi_I(x,y,z,t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[D_{\phi_I}(x,y,z,T) \frac{\partial \Phi_I(x,y,z,t)}{\partial y} \right] + \\ &+ \frac{\partial}{\partial z} \left[D_{\phi_I}(x,y,z,T) \frac{\partial \Phi_I(x,y,z,t)}{\partial z} \right] + k_{I,I}(x,y,z,T) I^2(x,y,z,t) - k_I(x,y,z,T) I(x,y,z,t) \end{aligned} \quad (6)$$

$$\begin{aligned} \frac{\partial \Phi_V(x,y,z,t)}{\partial t} &= \frac{\partial}{\partial x} \left[D_{\phi_V}(x,y,z,T) \frac{\partial \Phi_V(x,y,z,t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[D_{\phi_V}(x,y,z,T) \frac{\partial \Phi_V(x,y,z,t)}{\partial y} \right] + \\ &+ \frac{\partial}{\partial z} \left[D_{\phi_V}(x,y,z,T) \frac{\partial \Phi_V(x,y,z,t)}{\partial z} \right] + k_{V,V}(x,y,z,T) V^2(x,y,z,t) - k_V(x,y,z,T) V(x,y,z,t) \end{aligned}$$

with boundary and initial conditions

$$\begin{aligned} \left. \frac{\partial \Phi_\rho(x,y,z,t)}{\partial x} \right|_{x=0} &= 0, \left. \frac{\partial \Phi_\rho(x,y,z,t)}{\partial x} \right|_{x=L_x} = 0, \left. \frac{\partial \Phi_\rho(x,y,z,t)}{\partial y} \right|_{y=0} = 0, \left. \frac{\partial \Phi_\rho(x,y,z,t)}{\partial y} \right|_{y=L_y} = 0, \\ \left. \frac{\partial \Phi_\rho(x,y,z,t)}{\partial z} \right|_{z=0} &= 0, \left. \frac{\partial \Phi_\rho(x,y,z,t)}{\partial z} \right|_{z=L_z} = 0, \Phi_I(x,y,z,0)=f_{\phi_I}(x,y,z), \Phi_V(x,y,z,0)=f_{\phi_V}(x,y,z). \end{aligned} \quad (7)$$

Here $D_{\phi_I}(x,y,z,T)$ and $D_{\phi_V}(x,y,z,T)$ are diffusion coefficients of complexes of point radiation defects; $k_I(x,y,z,T)$ and $k_V(x,y,z,T)$ are parameters of decay of the complexes.

To determine spatio-temporal distributions of concentrations of complexes of radiation defects we used considered in Refs. [14,19] approach. Framework the approach we transform approximations of diffusion coefficients of complexes of point radiation defects to the following form: $D_\rho(x,y,z,T) = D_{0\rho} [1+\varepsilon_\rho g_\rho(x,y,z,T)]$ and $k_{I,V}(x,y,z,T)=k_{0I,V}[1+\zeta h(x,y,z,T)]$, where $D_{0\rho}$ and $k_{0I,V}$ are the average values of appropriate parameters, $0 \leq \varepsilon_{\rho V} < 1$, $0 \leq \zeta < 1$, $|g_\rho(x,y,z,T)| \leq 1$, $|h(x,y,z,T)| \leq 1$. Let us introduced the following dimensionless variables: $\tilde{\rho}(x,y,z,t) = \frac{\rho(x,y,z,t)}{\rho^*}$, $\chi = x/L_x$, $\eta = y/L_y$,

$$\psi = z/L_z, \quad \vartheta = t \sqrt{D_{0IV} D_{0VV}} \left(\frac{1}{L_x^2} + \frac{1}{L_y^2} + \frac{1}{L_z^2} \right), \quad \omega = k_{0I,V} (L_x^2 + L_y^2 + L_z^2) \sqrt{\frac{I^* V^*}{D_{0I} D_{0V}}}, \quad b_x = 1 + \frac{L_x^2}{L_y^2} + \frac{L_x^2}{L_z^2},$$

$b_y = 1 + \frac{L_y^2}{L_x^2} + \frac{L_y^2}{L_z^2}$, $b_z = 1 + \frac{L_z^2}{L_x^2} + \frac{L_z^2}{L_y^2}$. Using the above variables leads to transformation Eqs. (4) to the following form

$$\begin{aligned} \frac{\partial \tilde{I}(\chi, \eta, \psi, \vartheta)}{\partial \vartheta} &= \frac{1}{b_x} \sqrt{\frac{D_{0I}}{D_{0V}}} \frac{\partial}{\partial \chi} \left\{ [1 + \varepsilon_I g_I(\chi, \eta, \psi, T)] \frac{\partial \tilde{I}(\chi, \eta, \psi, \vartheta)}{\partial \chi} \right\} + \frac{1}{b_y} \sqrt{\frac{D_{0I}}{D_{0V}}} \times \\ &\times \frac{\partial}{\partial \eta} \left\{ [1 + \varepsilon_I g_I(\chi, \eta, \psi, T)] \frac{\partial \tilde{I}(\chi, \eta, \psi, \vartheta)}{\partial \eta} \right\} + \frac{1}{b_z} \frac{\partial}{\partial \psi} \left\{ [1 + \varepsilon_I g_I(\chi, \eta, \psi, T)] \frac{\partial \tilde{I}(\chi, \eta, \psi, \vartheta)}{\partial \psi} \right\} \times \\ &\times \sqrt{\frac{D_{0I}}{D_{0V}}} - \omega \sqrt{\frac{V^*}{I^*}} [1 + \varsigma h(\chi, \eta, \psi, T)] \tilde{I}(\chi, \eta, \psi, \vartheta) \tilde{V}(\chi, \eta, \psi, \vartheta) \quad (8) \\ \frac{\partial \tilde{V}(\chi, \eta, \psi, \vartheta)}{\partial \vartheta} &= \frac{1}{b_x} \sqrt{\frac{D_{0V}}{D_{0I}}} \frac{\partial}{\partial \chi} \left\{ [1 + \varepsilon_V g_V(\chi, \eta, \psi, T)] \frac{\partial \tilde{V}(\chi, \eta, \psi, \vartheta)}{\partial \chi} \right\} + \frac{1}{b_y} \sqrt{\frac{D_{0V}}{D_{0I}}} \times \\ &\times \frac{\partial}{\partial \eta} \left\{ [1 + \varepsilon_V g_V(\chi, \eta, \psi, T)] \frac{\partial \tilde{V}(\chi, \eta, \psi, \vartheta)}{\partial \eta} \right\} + \frac{\partial}{\partial \psi} \left\{ [1 + \varepsilon_V g_V(\chi, \eta, \psi, T)] \frac{\partial \tilde{V}(\chi, \eta, \psi, \vartheta)}{\partial \psi} \right\} \times \\ &\times \frac{1}{b_z} \sqrt{\frac{D_{0V}}{D_{0I}}} - \omega \sqrt{\frac{I^*}{V^*}} [1 + \varsigma h(\chi, \eta, \psi, T)] \tilde{I}(\chi, \eta, \psi, \vartheta) \tilde{V}(\chi, \eta, \psi, \vartheta). \end{aligned}$$

We will determine solution of Eqs. (8) as the following power series

$$\tilde{\rho}(\chi, \eta, \psi, \vartheta) = \sum_{i=0}^{\infty} \varepsilon_{\tilde{\rho}}^i \sum_{j=0}^{\infty} \omega^j \sum_{k=0}^{\infty} \varsigma^k \tilde{\rho}_{ijk}(\chi, \eta, \psi, \vartheta). \quad (9)$$

Substitution of the series into Eqs. (8) gives us possibility to obtain system of equations for initial-order approximations of concentrations of defects $\tilde{\rho}_{000}(\chi, \eta, \psi, \vartheta)$ and corrections for them $\tilde{\rho}_{ijk}(\chi, \eta, \psi, \vartheta)$ ($i \geq 1, j \geq 1, k \geq 1$). The equations are presented in Appendix.

Substitution of the series (9) into appropriate boundary and initial conditions gives us possibility to obtain boundary and initial conditions for the functions $\tilde{\rho}_{ijk}(\chi, \eta, \psi, \vartheta)$. The conditions dard approaches [21,22], are presented in Appendix. and solutions for the functions $\tilde{\rho}_{ijk}(\chi, \eta, \psi, \vartheta)$ ($i \geq 0, j \geq 0, k \geq 0$), which have been obtained by stan

Farther we determine spatio-temporal distributions of concentrations of point radiation defects. To calculate the distributions we transform approximations of diffusion coefficients to the following form: $D_{\phi I}(x, y, z, T) = D_{0\phi I}[1 + \varepsilon_{\phi I} g_{\phi I}(x, y, z, T)]$, $D_{\phi V}(x, y, z, T) = D_{0\phi V}[1 + \varepsilon_{\phi V} g_{\phi V}(x, y, z, T)]$. In this situation Eqs. (6) will be transform to the following form

$$\begin{aligned} \frac{\partial \Phi_i(x, y, z, t)}{\partial t} &= \left(\frac{\partial}{\partial x} \left\{ [1 + \varepsilon_{\phi I} g_{\phi I}(x, y, z, T)] \frac{\partial \Phi_i(x, y, z, t)}{\partial x} \right\} + \frac{\partial}{\partial y} \left\{ [1 + \varepsilon_{\phi I} g_{\phi I}(x, y, z, T)] \times \right. \right. \\ &\times \left. \left. \frac{\partial \Phi_i(x, y, z, t)}{\partial y} \right\} D_{0\phi I} - k_i(x, y, z, T) I(x, y, z, t) + k_{i,I}(x, y, z, T) I^2(x, y, z, t) \right. \end{aligned}$$

$$\frac{\partial \Phi_v(x, y, z, t)}{\partial t} = \left(\frac{\partial}{\partial x} \left\{ [1 + \varepsilon_{\Phi v} g_{\Phi v}(x, y, z, T)] \frac{\partial \Phi_v(x, y, z, t)}{\partial x} \right\} + \frac{\partial}{\partial y} \left\{ [1 + \varepsilon_{\Phi v} g_{\Phi v}(x, y, z, T)] \times \right. \right. \\ \left. \left. \times \frac{\partial \Phi_v(x, y, z, t)}{\partial y} \right\} D_{0\Phi v} - k_v(x, y, z, T) V(x, y, z, t) + k_{v,v}(x, y, z, T) V^2(x, y, z, t) \right).$$

We determine solutions of these equations as the following power series

$$\Phi_\rho(x, y, z, t) = \sum_{i=0}^{\infty} \varepsilon_{\Phi \rho}^i \Phi_{\rho i}(x, y, z, t), \quad (10)$$

where $\rho = I, V$. Substitution of the series (10) into Eqs. (6) and appropriate boundary and initial conditions gives us possibility to obtain equations for initial-order approximations of concentrations of complexes of point radiation defects, corrections for them, boundary and initial conditions for all above functions. The equations, conditions and solutions, which have been obtained by standard approaches [21,22], are presented in the Appendix.

Analysis of spatio-temporal distributions of concentrations of radiation defects has been done by using the second-order approximations on parameters, which used in appropriate series, and have been defined more precisely by using numerical simulation.

Farther we determine solution of the Eq.(1). To calculate the solution we used the approach, which has been considered in [13,18]. Framework the approach we transform approximation of dopant diffusion coefficient $D_L(x,y,z,T)$ into following form: $D_L(x,y,z,T) = D_{0L}[1 + \varepsilon_L g_L(x,y,z,T)]$. We determine solution of the Eq.(1) as the following power series

$$C(x, t) = \sum_{i=0}^{\infty} \varepsilon_L^i \sum_{j=0}^{\infty} \xi^j C_{ij}(x, t). \quad (11)$$

Substitution of the series into Eq. (1) gives us possibility to obtain system of equations for initial-order approximation of dopant concentration $C_{00}(x,y,z,t)$ and corrections for them $C_{ij}(x,y,z,t)$ ($i \geq 1, j \geq 1$). Substitution of the series (11) into appropriate boundary and initial conditions for the functions $C_{ij}(x,y,z,t)$ ($i \geq 0, j \geq 0$)

$$\left. \frac{\partial C_{ij}(x, y, z, t)}{\partial x} \right|_{x=0} = 0; \left. \frac{\partial C_{ij}(x, y, z, t)}{\partial x} \right|_{x=L_x} = 0; \left. \frac{\partial C_{ij}(x, y, z, t)}{\partial y} \right|_{y=0} = 0; \left. \frac{\partial C_{ij}(x, y, z, t)}{\partial y} \right|_{y=L_y} = 0; \\ \left. \frac{\partial C_{ij}(x, y, z, t)}{\partial z} \right|_{z=0} = 0; \left. \frac{\partial C_{ij}(x, y, z, t)}{\partial z} \right|_{z=L_z} = 0; C_{00}(x, y, z, 0) = f_C(x, y, z); C_{ij}(x, y, z, 0) = 0, i \geq 0, j \geq 0.$$

Solutions of equations for the functions $C_{ij}(x,y,z,t)$ ($i \geq 0, j \geq 0$), which has been calculated by standard approaches [21,22], are presented in the Appendix.

Analysis of spatio-temporal distribution of dopant concentration has been done analytically by using the second-order approximation on parameters, which has been used in appropriate series and have been defined more precisely by using numerical simulation.

3. Discussion

In this section we analyzed dynamics of redistribution of dopant with account relaxation of distributions of concentrations of radiation defects (in the case of ion doping of heterostructure). The Figs. 2 show distributions of concentrations of infused and implanted dopants in one of last epitaxial layers in direction, which is perpendicular to interfaces between epitaxial layers, after annealing of dopant and/or radiation defects, respectively. In this case values of dopant diffusion coefficient in last epitaxial layers is larger, than value of dopant diffusion coefficient in average epitaxial layer. The figures show, that interfaces between epitaxial layers under the above conditions give us possibility to increase sharpness of p - n -junctions and at the same time to increase homogeneity of distributions of concentrations of dopants in enriched by the dopants areas.

The Figs. 3 show distributions of concentrations of infused and implanted dopants in one of last epitaxial layers in direction, which is perpendicular to interfaces between epitaxial layers, after annealing of dopant and/or radiation defects, respectively. In this case values of dopant diffusion coefficient in last epitaxial layers is smaller, than value of dopant diffusion coefficient in average epitaxial layer. The figures show, that presents of last epitaxial layers leads to increasing of homogeneity of dopant in the average epitaxial layers. However sharpness of p - n -junctions decreases in comparison with p - n -junctions for Figs. 2. In this case one can obtain accelerated diffusion in last epitaxial layers. The decreasing of sharpness of p - n -junctions is a reason to use higher level of doping of last epitaxial layer to use nonlinearity of dopant diffusion. In this case one obtain n^+ - p - n^+ and/or p^+ - n - p^+ structures.

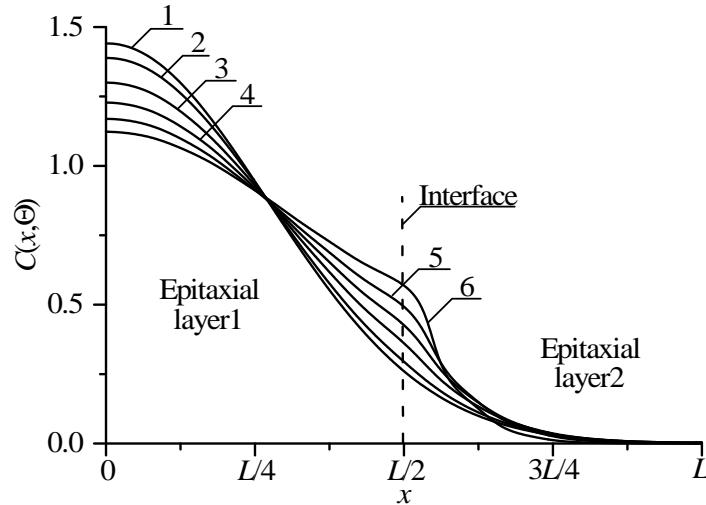


Fig. 2a. Distributions of concentrations of infused dopant in heterostructure from Fig. 1. Increasing of number of curves corresponds to increasing of difference between values of dopant diffusion coefficient

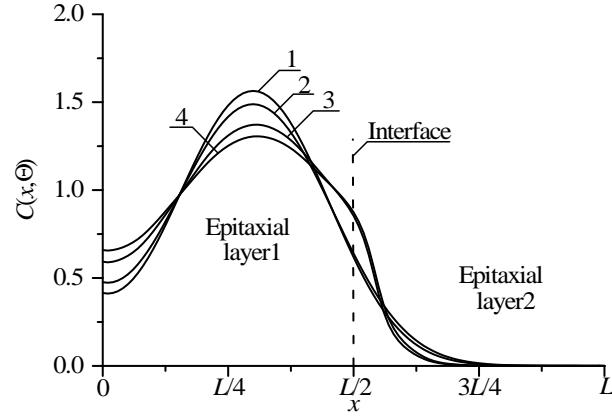


Fig. 2b. Distributions of concentrations of implanted dopant in heterostructure from Fig. 1. Increasing of number of curves corresponds to increasing of difference between values of dopant diffusion coefficient

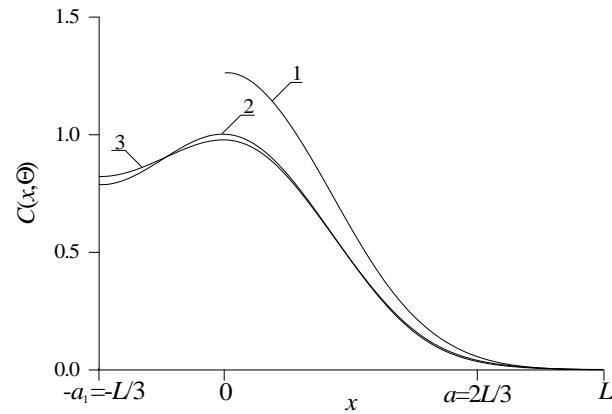


Fig. 3a. Distributions of concentration of infused in average epitaxial layer dopant in the heterostructure in Fig. 1 without another epitaxial layers (curve 1) and with them for the case, when dopant diffusion coefficient in the average epitaxial layer is smaller in comparison with dopant diffusion coefficients in another layers (curves 2 and 3). Increasing of number of curves corresponds to increasing of difference between values of dopant diffusion coefficients epitaxial layers of heterostructure

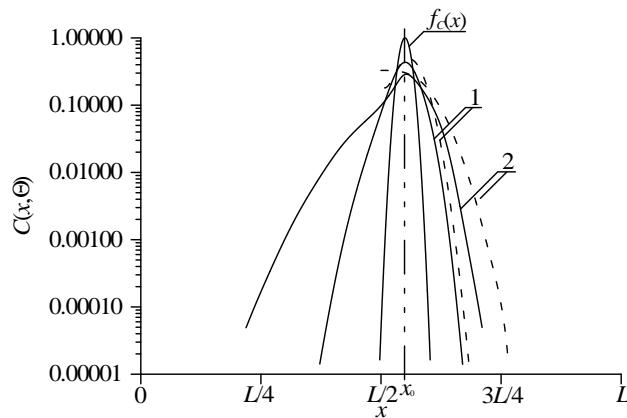


Fig. 3b. Distributions of concentration of implanted in average epitaxial layer dopant in the heterostructure in Fig. 1 without another epitaxial layers (curve 1) and with them for the case, when dopant diffusion coefficient in the average epitaxial layer is smaller in comparison with dopant diffusion coefficients in another layers (curves 2 and 3). Increasing of number of curves corresponds to increasing of difference between values of dopant diffusion coefficients epitaxial layers of heterostructure

Optimal value of annealing time we determine framework recently introduced criterion [12-14]. Framework the criterion we approximate real distributions of dopant by step-wise function and minimize the following mean-squared error

$$U = \frac{1}{L} \int_0^L [C(x, \Theta) - \psi(x)]^2 dx \quad (12)$$

at annealing time Θ . Dependences of the optimal value of annealing time from different parameters are presented on Figs. 4.

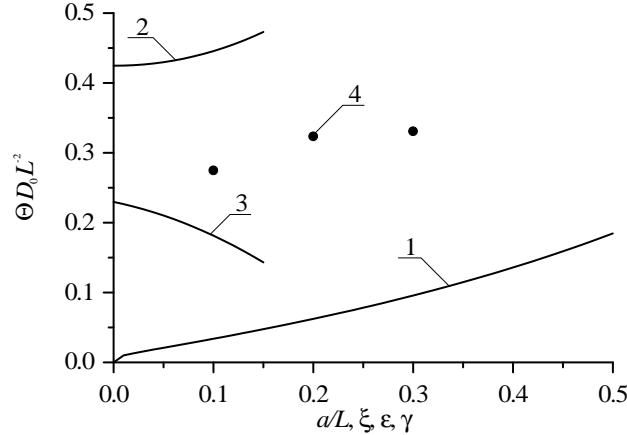


Fig. 4a. Dependences of dimensionless optimal value of annealing time of infused dopant, which has been calculated by minimization the mean-squared error (12), on different parameters of heterostructure. Curve 1 is the dependence of annealing time on relation $a/L, \xi=\gamma=0$ and equal to each other values of dopant diffusion coefficient in epitaxial layers. Curve 2 is the dependence of annealing time on parameter ξ for $a/L=1/2$ and $\xi=\gamma=0$. Curve 3 is the dependence of annealing time on parameter ξ for $a/L=1/2$ and $\xi=\gamma=0$. Curve 4 is the dependence of annealing time on parameter γ for $a/L=1/2$ and $\xi=\gamma=0$

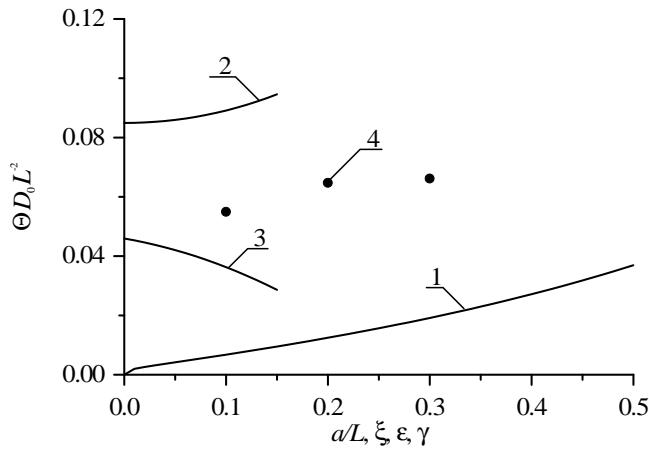


Fig. 4b. Dependences of dimensionless optimal value time of additional annealing of implanted dopant, which has been calculated by minimization the mean-squared error (12), on different parameters of heterostructure. Curve 1 is the dependence of annealing time on relation a/L , $\xi=\gamma=0$ and equal to each other values of dopant diffusion coefficient in epitaxial layers. Curve 2 is the dependence of annealing time on parameter ε for $a/L=1/2$ and $\xi=\gamma=0$. Curve 3 is the dependence of annealing time on parameter ξ for $a/L=1/2$ and $\varepsilon=\gamma=0$. Curve 4 is the dependence of annealing time on parameter γ for $a/L=1/2$ and $\varepsilon=\xi=0$

The figures show, that optimal values of annealing time after ion implantation are smaller, than optimal values of annealing time after infusion of dopant. Reason of the difference is necessity to use annealing of radiation defects after ion implantation. After that (if necessary) it could be used additional annealing of dopant. One can obtain spreading of distribution of concentration during annealing of radiation defects. Increasing of annealing time with increasing of thickness of epitaxial layer is the consequence of necessity of higher time for dopant to achieve interfaces between epitaxial layers of heterostructure. Decreasing of annealing time with increasing of values of parameters ε and ξ is the consequence of increasing of values of dopant diffusion coefficient in the area, where main part of dopant has been diffused. Increasing of annealing time with increasing of the parameter γ is the consequence of decreasing of the term $[C(x,y,z,t)/P(x,y,z,T)]^\gamma$ in approximation of dopant diffusion coefficient (3) with increasing of the parameter γ , because dopant concentration did not usually achieved value of limit of solubility of dopant and parameter γ is not smaller, than 1.

4. Conclusion

In this paper we introduce an approach of manufacturing multiemitter heterotransistors. Framework the approach the considered transistors became more compact and will include into itself p - n -junctions with higher sharpness.

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APPENDIX

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

$$\begin{aligned} \frac{\partial \tilde{I}_{000}(\chi, \eta, \psi, \vartheta)}{\partial \vartheta} &= \sqrt{\frac{D_{0I}}{D_{0V}}} \left[\frac{1}{b_x} \frac{\partial^2 \tilde{I}_{000}(\chi, \eta, \psi, \vartheta)}{\partial \chi^2} + \frac{1}{b_y} \frac{\partial^2 \tilde{I}_{000}(\chi, \eta, \psi, \vartheta)}{\partial \eta^2} + \frac{1}{b_z} \frac{\partial^2 \tilde{I}_{000}(\chi, \eta, \psi, \vartheta)}{\partial \psi^2} \right]; \\ \frac{\partial \tilde{V}_{000}(\chi, \eta, \psi, \vartheta)}{\partial \vartheta} &= \sqrt{\frac{D_{0V}}{D_{0I}}} \left[\frac{1}{b_x} \frac{\partial^2 \tilde{V}_{000}(\chi, \eta, \psi, \vartheta)}{\partial \chi^2} + \frac{1}{b_y} \frac{\partial^2 \tilde{V}_{000}(\chi, \eta, \psi, \vartheta)}{\partial \eta^2} + \frac{1}{b_z} \frac{\partial^2 \tilde{V}_{000}(\chi, \eta, \psi, \vartheta)}{\partial \psi^2} \right]; \\ \frac{\partial \tilde{I}_{i00}(\chi, \eta, \psi, \vartheta)}{\partial \vartheta} &= \sqrt{\frac{D_{0I}}{D_{0V}}} \left[\frac{1}{b_x} \frac{\partial^2 \tilde{I}_{i00}(\chi, \eta, \psi, \vartheta)}{\partial \chi^2} + \frac{1}{b_y} \frac{\partial^2 \tilde{I}_{i00}(\chi, \eta, \psi, \vartheta)}{\partial \eta^2} + \frac{1}{b_z} \frac{\partial^2 \tilde{I}_{i00}(\chi, \eta, \psi, \vartheta)}{\partial \psi^2} \right] + \\ &+ \sqrt{\frac{D_{0I}}{D_{0V}}} \left\{ \frac{1}{b_x} \frac{\partial}{\partial \chi} \left[g_i(\chi, \eta, \psi, T) \frac{\partial \tilde{I}_{i-100}(\chi, \eta, \psi, \vartheta)}{\partial \chi} \right] + \frac{1}{b_y} \frac{\partial}{\partial \eta} \left[g_i(\chi, \eta, \psi, T) \frac{\partial \tilde{I}_{i-100}(\chi, \eta, \psi, \vartheta)}{\partial \eta} \right] + \right. \end{aligned}$$

$$\begin{aligned}
 & + \frac{1}{b_z} \frac{\partial}{\partial \psi} \left[g_i(\chi, \eta, \psi, T) \frac{\partial \tilde{V}_{i-100}(\chi, \eta, \psi, \vartheta)}{\partial \psi} \right], i \geq 1; \\
 \frac{\partial \tilde{V}_{i00}(\chi, \eta, \psi, \vartheta)}{\partial \vartheta} &= \sqrt{\frac{D_{0V}}{D_{0I}}} \left[\frac{1}{b_x} \frac{\partial^2 \tilde{V}_{i00}(\chi, \eta, \psi, \vartheta)}{\partial \chi^2} + \frac{1}{b_y} \frac{\partial^2 \tilde{V}_{i00}(\chi, \eta, \psi, \vartheta)}{\partial \eta^2} + \frac{1}{b_z} \frac{\partial^2 \tilde{V}_{i00}(\chi, \eta, \psi, \vartheta)}{\partial \psi^2} \right] + \\
 & + \sqrt{\frac{D_{0V}}{D_{0I}}} \left\{ \frac{1}{b_x} \frac{\partial}{\partial \chi} \left[g_v(\chi, \eta, \psi, T) \frac{\partial \tilde{V}_{i-100}(\chi, \eta, \psi, \vartheta)}{\partial \chi} \right] + \frac{1}{b_y} \frac{\partial}{\partial \eta} \left[g_v(\chi, \eta, \psi, T) \frac{\partial \tilde{V}_{i-100}(\chi, \eta, \psi, \vartheta)}{\partial \eta} \right] + \right. \\
 & \quad \left. + \frac{1}{b_z} \frac{\partial}{\partial \psi} \left[g_v(\chi, \eta, \psi, T) \frac{\partial \tilde{V}_{i-100}(\chi, \eta, \psi, \vartheta)}{\partial \psi} \right] \right\}, i \geq 1; \\
 \frac{\partial \tilde{I}_{010}(\chi, \eta, \psi, \vartheta)}{\partial \vartheta} &= \sqrt{\frac{D_{0I}}{D_{0V}}} \left[\frac{1}{b_x} \frac{\partial^2 \tilde{I}_{010}(\chi, \eta, \psi, \vartheta)}{\partial \chi^2} + \frac{1}{b_y} \frac{\partial^2 \tilde{I}_{010}(\chi, \eta, \psi, \vartheta)}{\partial \eta^2} + \frac{1}{b_z} \frac{\partial^2 \tilde{I}_{010}(\chi, \eta, \psi, \vartheta)}{\partial \psi^2} \right] - \\
 & \quad - \sqrt{\frac{V^*}{I^*}} \tilde{I}_{000}(\chi, \eta, \psi, \vartheta) \tilde{V}_{000}(\chi, \eta, \psi, \vartheta); \\
 \frac{\partial \tilde{V}_{010}(\chi, \eta, \psi, \vartheta)}{\partial \vartheta} &= \sqrt{\frac{D_{0V}}{D_{0I}}} \left[\frac{1}{b_x} \frac{\partial^2 \tilde{V}_{010}(\chi, \eta, \psi, \vartheta)}{\partial \chi^2} + \frac{1}{b_y} \frac{\partial^2 \tilde{V}_{010}(\chi, \eta, \psi, \vartheta)}{\partial \eta^2} + \frac{1}{b_z} \frac{\partial^2 \tilde{V}_{010}(\chi, \eta, \psi, \vartheta)}{\partial \psi^2} \right] - \\
 & \quad - \sqrt{\frac{V^*}{I^*}} \tilde{I}_{000}(\chi, \eta, \psi, \vartheta) \tilde{V}_{000}(\chi, \eta, \psi, \vartheta); \\
 \frac{\partial \tilde{I}_{020}(\chi, \eta, \psi, \vartheta)}{\partial \vartheta} &= \sqrt{\frac{D_{0I}}{D_{0V}}} \left[\frac{1}{b_x} \frac{\partial^2 \tilde{I}_{020}(\chi, \eta, \psi, \vartheta)}{\partial \chi^2} + \frac{1}{b_y} \frac{\partial^2 \tilde{I}_{020}(\chi, \eta, \psi, \vartheta)}{\partial \eta^2} + \frac{1}{b_z} \frac{\partial^2 \tilde{I}_{020}(\chi, \eta, \psi, \vartheta)}{\partial \psi^2} \right] - \\
 & \quad - \sqrt{\frac{V^*}{I^*}} \tilde{I}_{010}(\chi, \eta, \psi, \vartheta) \tilde{V}_{000}(\chi, \eta, \psi, \vartheta) - \sqrt{\frac{V^*}{I^*}} \tilde{I}_{000}(\chi, \eta, \psi, \vartheta) \tilde{V}_{010}(\chi, \eta, \psi, \vartheta); \\
 \frac{\partial \tilde{V}_{020}(\chi, \eta, \psi, \vartheta)}{\partial \vartheta} &= \sqrt{\frac{D_{0V}}{D_{0I}}} \left[\frac{1}{b_x} \frac{\partial^2 \tilde{V}_{020}(\chi, \eta, \psi, \vartheta)}{\partial \chi^2} + \frac{1}{b_y} \frac{\partial^2 \tilde{V}_{020}(\chi, \eta, \psi, \vartheta)}{\partial \eta^2} + \frac{1}{b_z} \frac{\partial^2 \tilde{V}_{020}(\chi, \eta, \psi, \vartheta)}{\partial \psi^2} \right] - \\
 & \quad - \sqrt{\frac{I^*}{V^*}} \tilde{I}_{010}(\chi, \eta, \psi, \vartheta) \tilde{V}_{000}(\chi, \eta, \psi, \vartheta) - \sqrt{\frac{I^*}{V^*}} \tilde{I}_{000}(\chi, \eta, \psi, \vartheta) \tilde{V}_{010}(\chi, \eta, \psi, \vartheta); \\
 \frac{\partial \tilde{I}_{110}(\chi, \eta, \psi, \vartheta)}{\partial \vartheta} &= \sqrt{\frac{D_{0I}}{D_{0V}}} \left[\frac{1}{b_x} \frac{\partial^2 \tilde{I}_{110}(\chi, \eta, \psi, \vartheta)}{\partial \chi^2} + \frac{1}{b_y} \frac{\partial^2 \tilde{I}_{110}(\chi, \eta, \psi, \vartheta)}{\partial \eta^2} + \frac{1}{b_z} \frac{\partial^2 \tilde{I}_{110}(\chi, \eta, \psi, \vartheta)}{\partial \psi^2} \right] + \\
 & \quad + \sqrt{\frac{D_{0I}}{D_{0V}}} \left\{ \frac{1}{b_x} \frac{\partial}{\partial \chi} \left[g_i(\chi, \eta, \psi, T) \frac{\partial \tilde{I}_{010}(\chi, \eta, \psi, \vartheta)}{\partial \chi} \right] + \frac{1}{b_y} \frac{\partial}{\partial \eta} \left[g_i(\chi, \eta, \psi, T) \frac{\partial \tilde{I}_{010}(\chi, \eta, \psi, \vartheta)}{\partial \eta} \right] + \right. \\
 & \quad \left. + \frac{1}{b_z} \frac{\partial}{\partial \psi} \left[g_i(\chi, \eta, \psi, T) \frac{\partial \tilde{I}_{010}(\chi, \eta, \psi, \vartheta)}{\partial \psi} \right] \right\} - \sqrt{\frac{V^*}{I^*}} \tilde{I}_{100}(\chi, \eta, \psi, \vartheta) \tilde{V}_{000}(\chi, \eta, \psi, \vartheta) - \sqrt{\frac{V^*}{I^*}} \times \\
 & \quad \times \tilde{I}_{000}(\chi, \eta, \psi, \vartheta) \tilde{V}_{100}(\chi, \eta, \psi, \vartheta); \\
 \frac{\partial \tilde{V}_{110}(\chi, \eta, \psi, \vartheta)}{\partial \vartheta} &= \sqrt{\frac{D_{0V}}{D_{0I}}} \left[\frac{1}{b_x} \frac{\partial^2 \tilde{V}_{110}(\chi, \eta, \psi, \vartheta)}{\partial \chi^2} + \frac{1}{b_y} \frac{\partial^2 \tilde{V}_{110}(\chi, \eta, \psi, \vartheta)}{\partial \eta^2} + \frac{1}{b_z} \frac{\partial^2 \tilde{V}_{110}(\chi, \eta, \psi, \vartheta)}{\partial \psi^2} \right] + \\
 & \quad + \sqrt{\frac{D_{0V}}{D_{0I}}} \left\{ \frac{1}{b_x} \frac{\partial}{\partial \chi} \left[g_v(\chi, \eta, \psi, T) \frac{\partial \tilde{V}_{010}(\chi, \eta, \psi, \vartheta)}{\partial \chi} \right] + \frac{1}{b_y} \frac{\partial}{\partial \eta} \left[g_v(\chi, \eta, \psi, T) \frac{\partial \tilde{V}_{010}(\chi, \eta, \psi, \vartheta)}{\partial \eta} \right] + \right.
\end{aligned}$$

$$\begin{aligned}
 & + \frac{1}{b_z} \frac{\partial}{\partial \psi} \left[g_v(\chi, \eta, \psi, T) \frac{\partial \tilde{V}_{010}(\chi, \eta, \psi, \vartheta)}{\partial \psi} \right] - \sqrt{\frac{I^*}{I^*}} \tilde{I}_{100}(\chi, \eta, \psi, \vartheta) \tilde{V}_{000}(\chi, \eta, \psi, \vartheta) - \sqrt{\frac{I^*}{I^*}} \times \\
 & \quad \times \tilde{I}_{000}(\chi, \eta, \psi, \vartheta) \tilde{V}_{100}(\chi, \eta, \psi, \vartheta); \\
 \frac{\partial \tilde{I}_{00k}(\chi, \eta, \psi, \vartheta)}{\partial \vartheta} &= \sqrt{\frac{D_{0I}}{D_{0V}}} \left[\frac{1}{b_x} \frac{\partial^2 \tilde{I}_{00k}(\chi, \eta, \psi, \vartheta)}{\partial \chi^2} + \frac{1}{b_y} \frac{\partial^2 \tilde{I}_{00k}(\chi, \eta, \psi, \vartheta)}{\partial \eta^2} + \frac{1}{b_z} \frac{\partial^2 \tilde{I}_{00k}(\chi, \eta, \psi, \vartheta)}{\partial \psi^2} \right] \\
 \frac{\partial \tilde{V}_{00k}(\chi, \eta, \psi, \vartheta)}{\partial \vartheta} &= \sqrt{\frac{D_{0V}}{D_{0I}}} \left[\frac{1}{b_x} \frac{\partial^2 \tilde{V}_{00k}(\chi, \eta, \psi, \vartheta)}{\partial \chi^2} + \frac{1}{b_y} \frac{\partial^2 \tilde{V}_{00k}(\chi, \eta, \psi, \vartheta)}{\partial \eta^2} + \frac{1}{b_z} \frac{\partial^2 \tilde{V}_{00k}(\chi, \eta, \psi, \vartheta)}{\partial \psi^2} \right]; \\
 \frac{\partial \tilde{I}_{101}(\chi, \eta, \psi, \vartheta)}{\partial \vartheta} &= \sqrt{\frac{D_{0I}}{D_{0V}}} \left[\frac{1}{b_x} \frac{\partial^2 \tilde{I}_{101}(\chi, \eta, \psi, \vartheta)}{\partial \chi^2} + \frac{1}{b_y} \frac{\partial^2 \tilde{I}_{101}(\chi, \eta, \psi, \vartheta)}{\partial \eta^2} + \frac{1}{b_z} \frac{\partial^2 \tilde{I}_{101}(\chi, \eta, \psi, \vartheta)}{\partial \psi^2} \right] + \\
 & + \sqrt{\frac{D_{0I}}{D_{0V}}} \left\{ \frac{1}{b_x} \frac{\partial}{\partial \chi} \left[g_i(\chi, \eta, \psi, T) \frac{\partial \tilde{I}_{001}(\chi, \eta, \psi, \vartheta)}{\partial \chi} \right] + \frac{1}{b_y} \frac{\partial}{\partial \eta} \left[g_i(\chi, \eta, \psi, T) \frac{\partial \tilde{I}_{001}(\chi, \eta, \psi, \vartheta)}{\partial \eta} \right] + \right. \\
 & \quad \left. + \frac{1}{b_z} \frac{\partial}{\partial \psi} \left[g_i(\chi, \eta, \psi, T) \frac{\partial \tilde{I}_{001}(\chi, \eta, \psi, \vartheta)}{\partial \psi} \right] \right\}; \\
 \frac{\partial \tilde{V}_{101}(\chi, \vartheta)}{\partial \vartheta} &= \sqrt{\frac{D_{0V}}{D_{0I}}} \left[\frac{1}{b_x} \frac{\partial^2 \tilde{V}_{101}(\chi, \eta, \psi, \vartheta)}{\partial \chi^2} + \frac{1}{b_y} \frac{\partial^2 \tilde{V}_{101}(\chi, \eta, \psi, \vartheta)}{\partial \eta^2} + \frac{1}{b_z} \frac{\partial^2 \tilde{V}_{101}(\chi, \eta, \psi, \vartheta)}{\partial \psi^2} \right] + \\
 & + \sqrt{\frac{D_{0V}}{D_{0I}}} \left\{ \frac{1}{b_x} \frac{\partial}{\partial \chi} \left[g_v(\chi, \eta, \psi, T) \frac{\partial \tilde{I}_{001}(\chi, \eta, \psi, \vartheta)}{\partial \chi} \right] + \frac{1}{b_y} \frac{\partial}{\partial \eta} \left[g_v(\chi, \eta, \psi, T) \frac{\partial \tilde{I}_{001}(\chi, \eta, \psi, \vartheta)}{\partial \eta} \right] + \right. \\
 & \quad \left. + \frac{1}{b_z} \frac{\partial}{\partial \psi} \left[g_v(\chi, \eta, \psi, T) \frac{\partial \tilde{I}_{001}(\chi, \eta, \psi, \vartheta)}{\partial \psi} \right] \right\}; \\
 \frac{\partial \tilde{I}_{011}(\chi, \eta, \psi, \vartheta)}{\partial \vartheta} &= \sqrt{\frac{D_{0I}}{D_{0V}}} \left[\frac{1}{b_x} \frac{\partial^2 \tilde{I}_{011}(\chi, \eta, \psi, \vartheta)}{\partial \chi^2} + \frac{1}{b_y} \frac{\partial^2 \tilde{I}_{011}(\chi, \eta, \psi, \vartheta)}{\partial \eta^2} + \frac{1}{b_z} \frac{\partial^2 \tilde{I}_{011}(\chi, \eta, \psi, \vartheta)}{\partial \psi^2} \right] + \\
 & - \sqrt{\frac{V^*}{I^*}} \left[\tilde{I}_{001}(\chi, \eta, \psi, \vartheta) \tilde{V}_{000}(\chi, \eta, \psi, \vartheta) - h(\chi, \eta, \psi, T) \tilde{I}_{000}(\chi, \eta, \psi, \vartheta) \tilde{V}_{000}(\chi, \eta, \psi, \vartheta) - \right. \\
 & \quad \left. - \tilde{I}_{000}(\chi, \eta, \psi, \vartheta) \tilde{V}_{001}(\chi, \eta, \psi, \vartheta) \right] \\
 \frac{\partial \tilde{V}_{011}(\chi, \eta, \psi, \vartheta)}{\partial \vartheta} &= \sqrt{\frac{D_{0V}}{D_{0I}}} \left[\frac{1}{b_x} \frac{\partial^2 \tilde{V}_{011}(\chi, \eta, \psi, \vartheta)}{\partial \chi^2} + \frac{1}{b_y} \frac{\partial^2 \tilde{V}_{011}(\chi, \eta, \psi, \vartheta)}{\partial \eta^2} + \frac{1}{b_z} \frac{\partial^2 \tilde{V}_{011}(\chi, \eta, \psi, \vartheta)}{\partial \psi^2} \right] - \\
 & - \sqrt{\frac{V^*}{I^*}} \left[\tilde{I}_{001}(\chi, \eta, \psi, \vartheta) \tilde{V}_{000}(\chi, \eta, \psi, \vartheta) - h(\chi, \eta, \psi, T) \tilde{I}_{000}(\chi, \eta, \psi, \vartheta) \tilde{V}_{000}(\chi, \eta, \psi, \vartheta) - \right. \\
 & \quad \left. - \tilde{I}_{000}(\chi, \eta, \psi, \vartheta) \tilde{V}_{001}(\chi, \eta, \psi, \vartheta) \right]. \\
 \frac{\partial \tilde{\rho}_{ijk}(\chi, \eta, \psi, \vartheta)}{\partial \chi} \Big|_{\chi=0} &= 0; \quad \frac{\partial \tilde{\rho}_{ijk}(\chi, \eta, \psi, \vartheta)}{\partial \chi} \Big|_{\chi=1} = 0; \quad \frac{\partial \tilde{\rho}_{ijk}(\chi, \eta, \psi, \vartheta)}{\partial \eta} \Big|_{\eta=0} = 0; \quad \frac{\partial \tilde{\rho}_{ijk}(\chi, \eta, \psi, \vartheta)}{\partial \eta} \Big|_{\eta=1} = 0; \\
 \frac{\partial \tilde{\rho}_{ijk}(\chi, \eta, \psi, \vartheta)}{\partial \psi} \Big|_{\psi=0} &= 0; \quad \frac{\partial \tilde{\rho}_{ijk}(\chi, \eta, \psi, \vartheta)}{\partial \psi} \Big|_{\psi=1} = 0, \quad i \geq 1, j \geq 1, k \geq 1; \quad \tilde{\rho}_{000}(\chi, \eta, \psi, 0) = \frac{f_\rho(\chi, \eta, \psi)}{\rho^*}; \\
 \tilde{\rho}_{ijk}(\chi, \eta, \psi, 0) &= 0, \quad i \geq 1, j \geq 1, k \geq 1.
 \end{aligned}$$

Solutions of equations for the functions $\tilde{\rho}_{ijk}(\chi, \eta, \psi, \vartheta)$ ($i \geq 0, j \geq 0, k \geq 0$) could be written as

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

where $F_{n\rho} = \frac{1}{\rho^*} \int_0^1 c(u) \int_0^1 c(v) \int_0^1 c(w) f_{n\rho}(u, v, w) dw dv du$, $c_n(\alpha) = \cos(\pi n \alpha)$, $e_n(g) = \exp(-\pi^2 n^2 g \sqrt{D_{0v}/D_{0t}})$, $e_{nv}(g) = \exp(-\pi^2 n^2 g \sqrt{D_{0t}/D_{0v}})$;

$$\begin{aligned} \tilde{\rho}_{i00}(\chi, \eta, \psi, g) &= -\frac{2\pi D_{0\rho}}{b_x \rho * L_x^2 L_y L_z} \sum_{n=1}^{\infty} n c_n(\chi) c_n(\eta) c_n(\psi) e_{n\rho}(g) \int_0^2 e_{n\rho}(-\tau) \int_0^1 s_n(u) \int_0^1 c_n(v) \int_0^1 g_v(u, v, w, T) \times \\ &\quad \times c_n(w) \frac{\partial \tilde{\rho}_{i-100}(u, v, w, \tau)}{\partial u} dw dv du d\tau - \frac{2\pi D_{0\rho}}{b_y \rho * L_x L_y^2 L_z} \sum_{n=1}^{\infty} n c_n(\chi) c_n(\eta) c_n(\psi) e_{n\rho}(g) \int_0^2 e_{n\rho}(-\tau) \times \\ &\quad \times \int_0^1 c_n(u) \int_0^1 s_n(v) \int_0^1 c_n(w) g_v(u, v, w, T) \frac{\partial \tilde{\rho}_{i-100}(u, v, w, \tau)}{\partial v} dw dv du d\tau - \frac{2\pi D_{0\rho}}{b_z \rho * L_x L_y L_z^2} \sum_{n=1}^{\infty} n c_n(\chi) \times \\ &\quad \times c_n(\eta) c_n(\psi) e_{n\rho}(g) \int_0^2 e_{n\rho}(-\tau) \int_0^1 c_n(u) \int_0^1 c_n(v) \int_0^1 s_n(w) \frac{\partial \tilde{\rho}_{i-100}(u, v, w, \tau)}{\partial w} g_v(u, v, w, T) dw dv du d\tau, i \geq 1; \end{aligned}$$

$$\begin{aligned} \tilde{I}_{010}(\chi, \eta, \psi, g) &= -\frac{2D_{0t}}{I * L_x L_y L_z} \sqrt{\frac{V^*}{I^*}} \sum_{n=1}^{\infty} c_n(\chi) c_n(\eta) c_n(\psi) e_{nI}(g) \int_0^2 e_{nI}(-\tau) \int_0^1 c_n(u) \int_0^1 c_n(v) \int_0^1 c_n(w) \times \\ &\quad \times \tilde{I}_{000}(u, v, w, \tau) \tilde{V}_{000}(u, v, w, \tau) dw dv du d\tau; \end{aligned}$$

$$\begin{aligned} \tilde{V}_{010}(\chi, \eta, \psi, g) &= -\frac{2D_{0t}}{V * L_x L_y L_z} \sqrt{\frac{I^*}{V^*}} \sum_{n=1}^{\infty} c_n(\chi) c_n(\eta) c_n(\psi) e_{nV}(g) \int_0^2 e_{nV}(-\tau) \int_0^1 c_n(u) \int_0^1 c_n(v) \int_0^1 c_n(w) \times \\ &\quad \times \tilde{I}_{000}(u, v, w, \tau) \tilde{V}_{000}(u, v, w, \tau) dw dv du d\tau; \end{aligned}$$

$$\begin{aligned} \tilde{I}_{020}(\chi, \eta, \psi, g) &= -\frac{2D_{0t}}{I * L_x L_y L_z} \sqrt{\frac{V^*}{I^*}} \sum_{n=1}^{\infty} c_n(\chi) c_n(\eta) c_n(\psi) e_{nI}(g) \int_0^2 e_{nI}(-\tau) \int_0^1 c_n(u) \int_0^1 c_n(v) \int_0^1 c_n(w) \times \\ &\quad \times \tilde{I}_{010}(u, v, w, \tau) \tilde{V}_{000}(u, v, w, \tau) dw dv du d\tau - \frac{2D_{0t}}{I * L_x L_y L_z} \sqrt{\frac{V^*}{I^*}} \sum_{n=1}^{\infty} c_n(\chi) c_n(\eta) c_n(\psi) e_{nI}(g) \times \\ &\quad \times \int_0^2 e_{nI}(-\tau) \int_0^1 c_n(u) \int_0^1 c_n(v) \int_0^1 c_n(w) \tilde{I}_{000}(u, v, w, \tau) \tilde{V}_{010}(u, v, w, \tau) dw dv du d\tau; \end{aligned}$$

$$\begin{aligned} \tilde{V}_{020}(\chi, \eta, \psi, g) &= -\frac{2D_{0t}}{V * L_x L_y L_z} \sqrt{\frac{I^*}{V^*}} \sum_{n=1}^{\infty} c_n(\chi) c_n(\eta) c_n(\psi) e_{nV}(g) \int_0^2 e_{nV}(-\tau) \int_0^1 c_n(u) \int_0^1 c_n(v) \int_0^1 c_n(w) \times \\ &\quad \times \tilde{I}_{010}(u, v, w, \tau) \tilde{V}_{000}(u, v, w, \tau) dw dv du d\tau - \frac{2D_{0t}}{V * L_x L_y L_z} \sqrt{\frac{I^*}{V^*}} \sum_{n=1}^{\infty} c_n(\chi) c_n(\eta) c_n(\psi) e_{nV}(g) \times \\ &\quad \times \int_0^2 e_{nV}(-\tau) \int_0^1 c_n(u) \int_0^1 c_n(v) \int_0^1 c_n(w) \tilde{I}_{000}(u, v, w, \tau) \tilde{V}_{010}(u, v, w, \tau) dw dv du d\tau; \end{aligned}$$

$$\tilde{I}_{001}(\chi, \eta, \psi, g) = \tilde{I}_{002}(\chi, \eta, \psi, g) = \tilde{V}_{001}(\chi, \eta, \psi, g) = \tilde{V}_{002}(\chi, \eta, \psi, g) = 0;$$

$$\begin{aligned} \tilde{I}_{110}(\chi, \eta, \psi, g) &= \frac{2\pi D_{0t}}{b_x I * L_x^2 L_y L_z} \sqrt{\frac{V^*}{I^*}} \sum_{n=1}^{\infty} n c_n(\chi) c_n(\eta) c_n(\psi) e_{nI}(g) \int_0^2 e_{nI}(-\tau) \int_0^1 s_n(u) \int_0^1 c_n(v) \int_0^1 c_n(w) \times \\ &\quad \times g_i(u, v, w, T) \frac{\partial \tilde{I}_{010}(u, v, w, \tau)}{\partial u} dw dv du d\tau + \frac{2\pi D_{0t}}{b_y I * L_x L_y^2 L_z} \sqrt{\frac{V^*}{I^*}} \sum_{n=1}^{\infty} c_n(\chi) c_n(\eta) c_n(\psi) e_{nI}(g) \times \\ &\quad \times n \int_0^2 e_{nI}(-\tau) \int_0^1 c_n(u) \int_0^1 s_n(v) \int_0^1 c_n(w) g_i(u, v, w, T) \frac{\partial \tilde{I}_{010}(u, v, w, \tau)}{\partial v} dw dv du d\tau + \frac{2\pi D_{0t}}{b_z I * L_x L_y L_z^2} \times \end{aligned}$$

$$\begin{aligned}
 & \times \sqrt{\frac{V^*}{I^*}} \sum_{n=1}^{\infty} n c_n(\chi) c_n(\eta) \int_0^{\vartheta} e_{nI}(-\tau) \int_0^1 c_n(u) \int_0^1 c_n(v) \int_0^1 s_n(w) g_I(u, v, w, T) \frac{\partial \tilde{I}_{010}(u, v, w, \tau)}{\partial w} d w d v d u d \tau \times \\
 & \times c_n(\psi) e_{nI}(\vartheta) - \frac{2 D_{0I}}{I^* L_x L_y L_z} \sqrt{\frac{V^*}{I^*}} \sum_{n=1}^{\infty} c_n(\chi) c_n(\eta) c_n(\psi) e_{nI}(\vartheta) \int_0^{\vartheta} e_{nI}(-\tau) \int_0^1 c_n(u) \int_0^1 c_n(v) \int_0^1 \tilde{I}_{100}(u, v, w, \tau) \times \\
 & \times c_n(w) \tilde{V}_{000}(u, v, w, \tau) d w d v d u d \tau - \frac{2 D_{0I}}{I^* L^*} \sqrt{\frac{V^*}{I^*}} \sum_{n=1}^{\infty} c_n(\psi) e_{nI}(\vartheta) \int_0^{\vartheta} e_{nI}(-\tau) \int_0^1 c_n(u) \int_0^1 c_n(v) \int_0^1 c_n(w) \times \\
 & \times \tilde{I}_{000}(u, v, w, \tau) \tilde{V}_{100}(u, v, w, \tau) d w d v d u d \tau c_n(\chi) c_n(\eta); \\
 \tilde{V}_{110}(\chi, \eta, \psi, \vartheta) = & \frac{2 \pi D_{0V}}{b_x I^* L_x^2 L_y L_z} \sqrt{\frac{I^*}{V^*}} \sum_{n=1}^{\infty} n c_n(\chi) c_n(\eta) c_n(\psi) e_{nV}(\vartheta) \int_0^{\vartheta} e_{nV}(-\tau) \int_0^1 s_n(u) \int_0^1 c_n(v) \int_0^1 c_n(w) \times \\
 & \times g_V(u, v, w, T) \frac{\partial \tilde{V}_{010}(u, v, w, \tau)}{\partial u} d w d v d u d \tau + \frac{2 \pi D_{0V}}{b_y V^* L_x L_y^2 L_z} \sqrt{\frac{I^*}{V^*}} \sum_{n=1}^{\infty} n c_n(\chi) c_n(\eta) c_n(\psi) e_{nV}(\vartheta) \times \\
 & \times \int_0^{\vartheta} e_{nV}(-\tau) \int_0^1 c_n(u) \int_0^1 s_n(v) \int_0^1 c_n(w) g_V(u, v, w, T) \frac{\partial \tilde{V}_{010}(u, v, w, \tau)}{\partial v} d w d v d u d \tau + \frac{2 \pi D_{0V}}{b_z V^* L_x L_y L_z^2} \sqrt{\frac{I^*}{V^*}} \times \\
 & \times \sum_{n=1}^{\infty} n c_n(\chi) c_n(\eta) c_n(\psi) \int_0^{\vartheta} e_{nV}(-\tau) \int_0^1 c_n(u) \int_0^1 c_n(v) \int_0^1 s_n(w) g_V(u, v, w, T) \frac{\partial \tilde{V}_{010}(u, v, w, \tau)}{\partial w} d w d v d u d \tau \times \\
 & \times e_{nV}(\vartheta) - \frac{2 D_{0V}}{V^* L_x^2 L_y L_z} \sum_{n=1}^{\infty} c_n(\chi) e_{nV}(\vartheta) \int_0^{\vartheta} e_{nV}(-\tau) \int_0^1 c_n(v) \tilde{I}_{100}(u, v, w, \tau) \tilde{V}_{000}(u, v, w, \tau) d w d v d u d \tau \times \\
 & \times c_n(\eta) c_n(\psi) \sqrt{\frac{I^*}{V^*}} - \frac{2 D_{0V}}{V^* L^*} \sqrt{\frac{I^*}{V^*}} \sum_{n=1}^{\infty} c_n(\chi) c_n(\eta) c_n(\psi) \int_0^{\vartheta} e_{nV}(-\tau) \int_0^1 c_n(u) \int_0^1 c_n(v) \int_0^1 c_n(w) \tilde{I}_{000}(u, v, w, \tau) \times \\
 & \times \tilde{V}_{100}(u, v, w, \tau) d w d v d u d \tau e_{nV}(\vartheta); \\
 \tilde{I}_{101}(\chi, \eta, \psi, \vartheta) = & \frac{2 \pi}{b_x I^* L_x^2 L_y L_z} \sum_{n=1}^{\infty} n c_n(\chi) c_n(\eta) c_n(\psi) e_{nI}(\vartheta) \int_0^{\vartheta} e_{nI}(-\tau) \int_0^1 s_n(u) \int_0^1 c_n(v) \int_0^1 g_I(u, v, w, T) \times \\
 & \times c_n(w) \frac{\partial \tilde{I}_{001}(u, v, w, \tau)}{\partial u} d w d v d u d \tau + \frac{2 \pi}{b_y I^* L_x L_y^2 L_z} \sum_{n=1}^{\infty} c_n(\chi) c_n(\eta) c_n(\psi) e_{nI}(\vartheta) \int_0^{\vartheta} e_{nI}(-\tau) \int_0^1 c_n(u) \times \\
 & \times n \int_0^1 s_n(v) \int_0^1 c_n(w) g_I(u, v, w, T) \frac{\partial \tilde{I}_{001}(u, v, w, \tau)}{\partial v} d w d v d u d \tau + \frac{2 \pi}{b_z I^*} \sum_{n=1}^{\infty} n c_n(\chi) c_n(\eta) c_n(\psi) e_{nI}(\vartheta) \times \\
 & \times \int_0^{\vartheta} e_{nI}(-\tau) \int_0^1 c_n(u) \int_0^1 c_n(v) \int_0^1 s_n(w) g_I(u, v, w, T) \frac{\partial \tilde{I}_{001}(u, v, w, \tau)}{\partial w} d w d v d u d \tau \frac{1}{L_x L_y L_z^2}; \\
 \tilde{V}_{101}(\chi, \eta, \psi, \vartheta) = & \frac{2 \pi}{b_x V^* L_x^2 L_y L_z} \sum_{n=1}^{\infty} c_n(\chi) c_n(\eta) c_n(\psi) e_{nV}(\vartheta) \int_0^{\vartheta} e_{nV}(-\tau) \int_0^1 s_n(u) \int_0^1 c_n(v) \int_0^1 g_V(u, v, w, T) \times \\
 & \times n c_n(w) \frac{\partial \tilde{V}_{001}(u, v, w, \tau)}{\partial u} d w d v d u d \tau + \frac{2 \pi}{L_x L_y^2 L_z b_y} \sum_{n=1}^{\infty} n c_n(\chi) c_n(\eta) c_n(\psi) e_{nV}(\vartheta) \int_0^{\vartheta} e_{nV}(-\tau) \times \\
 & \times \int_0^1 c_n(u) \int_0^1 s_n(v) \int_0^1 c_n(w) g_V(u, v, w, T) \frac{\partial \tilde{V}_{001}(u, v, w, \tau)}{\partial v} d w d v d u d \tau + \frac{2 \pi}{b_z V^* L_x L_y L_z^2} \sum_{n=1}^{\infty} n c_n(\chi) \times \\
 & \times c_n(\eta) c_n(\psi) e_{nV}(\vartheta) \int_0^{\vartheta} e_{nV}(-\tau) \int_0^1 c_n(u) \int_0^1 c_n(v) \int_0^1 s_n(w) g_V(u, v, w, T) \frac{\partial \tilde{V}_{001}(u, v, w, \tau)}{\partial w} d w d v d u d \tau; \\
 \tilde{I}_{011}(\chi, \eta, \psi, \vartheta) = & - \frac{2}{I^* L_x L_y L_z} \sum_{n=1}^{\infty} c_n(\chi) c_n(\eta) c_n(\psi) e_{nI}(\vartheta) \int_0^{\vartheta} e_{nI}(-\tau) \int_0^1 c_n(u) \int_0^1 c_n(v) \int_0^1 \tilde{I}_{001}(u, v, w, \tau) \times
 \end{aligned}$$

$$\begin{aligned}
 & \times c_n(w) \tilde{V}_{000}(u, v, w, \tau) dwdvdud\tau \sqrt{\frac{V^*}{I^*}} - \frac{2}{I^* L_x L_y L_z} \sqrt{\frac{V^*}{I^*}} \sum_{n=1}^{\infty} c_n(\chi) c_n(\eta) c_n(\psi) e_{nI}^g(\vartheta) \int_0^{\vartheta} e_{nI}(-\tau) \times \\
 & \times \int_0^1 c_n(u) \int_0^1 c_n(v) \int_0^1 c_n(w) \tilde{I}_{000}(u, v, w, \tau) \tilde{V}_{001}(u, v, w, \tau) dwdvdud\tau - \frac{2}{L_x L_y L_z I^*} \sqrt{\frac{V^*}{I^*}} \sum_{n=1}^{\infty} c_n(\chi) c_n(\eta) \times \\
 & \times c_n(\psi) e_{nI}^g(\vartheta) \int_0^{\vartheta} e_{nI}(-\tau) \int_0^1 c_n(u) \int_0^1 c_n(v) \int_0^1 h(u, v, w, T) c_n(w) \tilde{I}_{000}(u, v, w, \tau) \tilde{V}_{001}(u, v, w, \tau) dwdvdud\tau ; \\
 \tilde{V}_{001}(\chi, \eta, \psi, \vartheta) = & - \frac{2}{V^* L_x L_y L_z} \sqrt{\frac{I^*}{V^*}} \sum_{n=1}^{\infty} c_n(\chi) c_n(\eta) c_n(\psi) e_{nV}^g(\vartheta) \int_0^{\vartheta} e_{nV}(-\tau) \int_0^1 c_n(u) \int_0^1 c_n(v) \int_0^1 c_n(w) \times \\
 & \times \tilde{I}_{001}(u, v, w, \tau) \tilde{V}_{000}(u, v, w, \tau) dwdvdud\tau - \frac{2}{V^* L_x L_y L_z} \sum_{n=1}^{\infty} c_n(\chi) c_n(\eta) c_n(\psi) e_{nV}^g(\vartheta) \int_0^{\vartheta} e_{nV}(-\tau) \times \\
 & \times \sqrt{\frac{I^*}{V^*}} \int_0^1 c_n(u) \int_0^1 c_n(v) \int_0^1 c_n(w) \tilde{I}_{000}(u, v, w, \tau) \tilde{V}_{001}(u, v, w, \tau) dwdvdud\tau - \frac{2}{V^* L_x L_y L_z} \sum_{n=1}^{\infty} c_n(\chi) \times \\
 & \times \sqrt{\frac{I^*}{V^*}} \int_0^{\vartheta} e_{nV}(-\tau) \int_0^1 c_n(u) \int_0^1 c_n(v) \int_0^1 h(u, v, w, T) c_n(w) \tilde{I}_{000}(u, v, w, \tau) \tilde{V}_{001}(u, v, w, \tau) dwdvdud\tau \times \\
 & \times c_n(\eta) c_n(\psi) e_{nV}^g(\vartheta).
 \end{aligned}$$

Equations for the functions $\Phi_{\rho i}(x, y, z, t)$ are

$$\begin{aligned}
 \frac{\partial \Phi_{i0}(x, y, z, t)}{\partial t} = & D_{0\Phi I} \left[\frac{\partial^2 \Phi_{i0}(x, y, z, t)}{\partial x^2} + \frac{\partial^2 \Phi_{i0}(x, y, z, t)}{\partial y^2} + \frac{\partial^2 \Phi_{i0}(x, y, z, t)}{\partial z^2} \right] + \\
 & + k_{i,I}(x, y, z, T) I^2(x, y, z, t) - k_i(x, y, z, T) I(x, y, z, t); \\
 \frac{\partial \Phi_{v0}(x, y, z, t)}{\partial t} = & D_{0\Phi V} \left[\frac{\partial^2 \Phi_{v0}(x, y, z, t)}{\partial x^2} + \frac{\partial^2 \Phi_{v0}(x, y, z, t)}{\partial y^2} + \frac{\partial^2 \Phi_{v0}(x, y, z, t)}{\partial z^2} \right] + \\
 & + k_{v,V}(x, y, z, T) V^2(x, y, z, t) - k_v(x, y, z, T) V(x, y, z, t); \\
 \frac{\partial \Phi_{ii}(x, y, z, t)}{\partial t} = & D_{0\Phi I} \frac{\partial^2 \Phi_{ii}(x, y, z, t)}{\partial x^2} + D_{0\Phi I} \frac{\partial^2 \Phi_{ii}(x, y, z, t)}{\partial y^2} + D_{0\Phi I} \frac{\partial^2 \Phi_{ii}(x, y, z, t)}{\partial z^2} + \\
 & + D_{0\Phi I} \frac{\partial}{\partial x} \left[g_{\Phi I}(x, y, z, T) \frac{\partial \Phi_{ii-1}(x, y, z, t)}{\partial x} \right] + D_{0\Phi I} \frac{\partial}{\partial y} \left[g_{\Phi I}(x, y, z, T) \frac{\partial \Phi_{ii-1}(x, y, z, t)}{\partial y} \right] + \\
 & + D_{0\Phi I} \frac{\partial}{\partial z} \left[g_{\Phi I}(x, y, z, T) \frac{\partial \Phi_{ii-1}(x, y, z, t)}{\partial z} \right], i \geq 1; \\
 \frac{\partial \Phi_{vi}(x, y, z, t)}{\partial t} = & D_{0\Phi V} \frac{\partial^2 \Phi_{vi}(x, y, z, t)}{\partial x^2} + D_{0\Phi V} \frac{\partial^2 \Phi_{vi}(x, y, z, t)}{\partial y^2} + D_{0\Phi V} \frac{\partial^2 \Phi_{vi}(x, y, z, t)}{\partial z^2} + \\
 & + D_{0\Phi V} \frac{\partial}{\partial x} \left[g_{\Phi V}(x, y, z, T) \frac{\partial \Phi_{vi-1}(x, y, z, t)}{\partial x} \right] + D_{0\Phi V} \frac{\partial}{\partial y} \left[g_{\Phi V}(x, y, z, T) \frac{\partial \Phi_{vi-1}(x, y, z, t)}{\partial y} \right] + \\
 & + D_{0\Phi V} \frac{\partial}{\partial z} \left[g_{\Phi V}(x, y, z, T) \frac{\partial \Phi_{vi-1}(x, y, z, t)}{\partial z} \right], i \geq 1; \\
 \left. \frac{\partial \Phi_{\rho i}(x, y, z, t)}{\partial x} \right|_{x=0} = & 0, \quad \left. \frac{\partial \Phi_{\rho i}(x, y, z, t)}{\partial x} \right|_{x=L_x} = 0, \quad \left. \frac{\partial \Phi_{\rho i}(x, y, z, t)}{\partial y} \right|_{y=0} = 0, \quad \left. \frac{\partial \Phi_{\rho i}(x, y, z, t)}{\partial y} \right|_{y=L_y} = 0, \\
 \left. \frac{\partial \Phi_{\rho i}(x, y, z, t)}{\partial z} \right|_{z=0} = & 0, \quad \left. \frac{\partial \Phi_{\rho i}(x, y, z, t)}{\partial z} \right|_{z=L_z} = 0, \quad i \geq 0; \quad \Phi_{i0}(x, y, z, 0) = f_{\Phi I}(x, y, z), \quad \Phi_{ii}(x, y, z, 0) = 0,
 \end{aligned}$$

$$\Phi_{V0}(x,y,z,0)=f_{\phi V}(x,y,z), \Phi_{Vi}(x,y,z,0)=0, i \geq 1.$$

Solutions of the equations could be written as

$$\Phi_{\rho 0}(x,y,z,t) = \frac{1}{L_x L_y L_z} + \frac{2}{L_x L_y L_z} \sum_{n=1}^{\infty} F_{n\Phi_{\rho}} c(x)c(y)c(z)e_{n\Phi_{\rho}}(t),$$

$$\text{where } e_{n\Phi_{\rho}}(t) = \exp\left[-\pi^2 n^2 D_{0\Phi_{\rho}} t \left(\frac{1}{L_x^2} + \frac{1}{L_y^2} + \frac{1}{L_z^2}\right)\right], \quad F_{n\Phi_{\rho}} = \int_0^{L_x} c_n(x) \int_0^{L_y} c_n(y) \int_0^{L_z} c_n(z) f_{\Phi_{\rho}}(x,y,z) dz dy dx,$$

$$c_n(\alpha) = \cos(\pi n \alpha / L_{\alpha});$$

$$\begin{aligned} \Phi_{\rho i}(x,y,z,t) = & -\frac{2\pi}{L_x^2 L_y L_z} \sum_{n=1}^{\infty} n c_n(x) c_n(y) c_n(z) e_{\Phi_{\rho^n}}(t) \int_0^t e_{\Phi_{\rho^n}}(-\tau) \int_0^{L_x} s_n(u) \int_0^{L_y} c_n(v) \int_0^{L_z} c_n(w) g_{\Phi_{\rho}}(u,v,w,T) \times \\ & \times \frac{\partial \Phi_{\rho^{i-1}}(u,v,w,\tau)}{\partial u} dw dv du d\tau - \frac{2\pi}{L_x L_y^2 L_z} \sum_{n=1}^{\infty} n c_n(x) c_n(y) c_n(z) e_{\Phi_{\rho^n}}(t) \int_0^t e_{\Phi_{\rho^n}}(-\tau) \int_0^{L_x} c_n(u) \int_0^{L_y} s_n(v) \times \\ & \times \int_0^{L_z} c_n(w) g_{\Phi_{\rho}}(u,v,w,T) \frac{\partial \Phi_{\rho^{i-1}}(u,v,w,\tau)}{\partial v} dw dv du d\tau - \frac{2\pi}{L_x L_y L_z^2} \sum_{n=1}^{\infty} n c_n(x) c_n(y) c_n(z) e_{\Phi_{\rho^n}}(t) \times \\ & \times \int_0^t e_{\Phi_{\rho^n}}(-\tau) \int_0^{L_x} c_n(u) \int_0^{L_y} c_n(v) \int_0^{L_z} s_n(w) g_{\Phi_{\rho}}(u,v,w,T) \frac{\partial \Phi_{\rho^{i-1}}(u,v,w,\tau)}{\partial w} dw dv du d\tau, \quad i \geq 1, \end{aligned}$$

$$\text{where } s_n(\alpha) = \sin(\pi n \alpha / L_{\alpha}).$$

System of equations for functions $C_{ijk}(x,y,z,t)$ ($i \geq 0, j \geq 0, k \geq 0$) could be written as

$$\begin{aligned} \frac{\partial C_{00}(x,y,z,t)}{\partial t} = & D_{0L} \left[\frac{\partial^2 C_{00}(x,y,z,t)}{\partial x^2} + \frac{\partial^2 C_{00}(x,y,z,t)}{\partial y^2} + \frac{\partial^2 C_{00}(x,y,z,t)}{\partial z^2} \right]; \\ \frac{\partial C_{i0}(x,y,z,t)}{\partial t} = & D_{0L} \frac{\partial^2 C_{i0}(x,y,z,t)}{\partial x^2} + D_{0L} \frac{\partial^2 C_{i0}(x,y,z,t)}{\partial y^2} + D_{0L} \frac{\partial^2 C_{i0}(x,y,z,t)}{\partial z^2} + \\ & + D_{0L} \frac{\partial}{\partial x} \left[g_L(x,y,z,T) \frac{\partial C_{i-10}(x,y,z,t)}{\partial x} \right] + D_{0L} \frac{\partial}{\partial y} \left[g_L(x,y,z,T) \frac{\partial C_{i-10}(x,y,z,t)}{\partial y} \right] + \\ & + D_{0L} \frac{\partial}{\partial z} \left[g_L(x,y,z,T) \frac{\partial C_{i-10}(x,y,z,t)}{\partial z} \right], \quad i \geq 1; \\ \frac{\partial C_{01}(x,y,z,t)}{\partial t} = & D_{0L} \frac{\partial^2 C_{01}(x,y,z,t)}{\partial x^2} + D_{0L} \frac{\partial^2 C_{01}(x,y,z,t)}{\partial y^2} + D_{0L} \frac{\partial^2 C_{01}(x,y,z,t)}{\partial z^2} + \\ & + D_{0L} \frac{\partial}{\partial x} \left[\frac{C_{00}^{\gamma}(x,y,z,t)}{P^{\gamma}(x,y,z,T)} \frac{\partial C_{00}(x,y,z,t)}{\partial x} \right] + D_{0L} \frac{\partial}{\partial y} \left[\frac{C_{00}^{\gamma}(x,y,z,t)}{P^{\gamma}(x,y,z,T)} \frac{\partial C_{00}(x,y,z,t)}{\partial y} \right] + \\ & + D_{0L} \frac{\partial}{\partial z} \left[\frac{C_{00}^{\gamma}(x,y,z,t)}{P^{\gamma}(x,y,z,T)} \frac{\partial C_{00}(x,y,z,t)}{\partial z} \right]; \\ \frac{\partial C_{02}(x,y,z,t)}{\partial t} = & D_{0L} \frac{\partial^2 C_{02}(x,y,z,t)}{\partial x^2} + D_{0L} \frac{\partial^2 C_{02}(x,y,z,t)}{\partial y^2} + D_{0L} \frac{\partial^2 C_{02}(x,y,z,t)}{\partial z^2} + D_{0L} \times \\ & \times \left\{ \frac{\partial}{\partial x} \left[C_{01}(x,y,z,t) \frac{C_{00}^{\gamma-1}(x,y,z,t)}{P^{\gamma}(x,y,z,T)} \frac{\partial C_{00}(x,y,z,t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[C_{01}(x,y,z,t) \frac{C_{00}^{\gamma-1}(x,y,z,t)}{P^{\gamma}(x,y,z,T)} \frac{\partial C_{00}(x,y,z,t)}{\partial y} \right] + \right. \end{aligned}$$

$$\begin{aligned}
 & + \frac{\partial}{\partial z} \left[C_{01}(x, y, z, t) \frac{C_{00}^{\gamma-1}(x, y, z, t)}{P^\gamma(x, y, z, T)} \frac{\partial C_{00}(x, y, z, t)}{\partial z} \right] + D_{0L} \left\{ \frac{\partial}{\partial x} \left[\frac{C_{00}^{\gamma}(x, y, z, t)}{P^\gamma(x, y, z, T)} \frac{\partial C_{01}(x, y, z, t)}{\partial x} \right] \right. \\
 & \quad \left. + \frac{\partial}{\partial y} \left[\frac{C_{00}^{\gamma}(x, y, z, t)}{P^\gamma(x, y, z, T)} \frac{\partial C_{01}(x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[\frac{C_{00}^{\gamma}(x, y, z, t)}{P^\gamma(x, y, z, T)} \frac{\partial C_{01}(x, y, z, t)}{\partial z} \right] \right\}; \\
 & \frac{\partial C_{11}(x, y, z, t)}{\partial t} = D_{0L} \frac{\partial^2 C_{11}(x, y, z, t)}{\partial x^2} + D_{0L} \frac{\partial^2 C_{11}(x, y, z, t)}{\partial y^2} + D_{0L} \frac{\partial^2 C_{11}(x, y, z, t)}{\partial z^2} + D_{0L} \times \\
 & \times \left\{ \frac{\partial}{\partial x} \left[C_{10}(x, y, z, t) \frac{C_{00}^{\gamma-1}(x, y, z, t)}{P^\gamma(x, y, z, T)} \frac{\partial C_{00}(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[C_{10}(x, y, z, t) \frac{C_{00}^{\gamma-1}(x, y, z, t)}{P^\gamma(x, y, z, T)} \frac{\partial C_{00}(x, y, z, t)}{\partial y} \right] + \right. \\
 & \quad \left. + \frac{\partial}{\partial z} \left[C_{10}(x, y, z, t) \frac{C_{00}^{\gamma-1}(x, y, z, t)}{P^\gamma(x, y, z, T)} \frac{\partial C_{00}(x, y, z, t)}{\partial z} \right] \right\} + D_{0L} \left\{ \frac{\partial}{\partial x} \left[\frac{C_{00}^{\gamma}(x, y, z, t)}{P^\gamma(x, y, z, t)} \frac{\partial C_{10}(x, y, z, t)}{\partial x} \right] + \right. \\
 & \quad \left. + \frac{\partial}{\partial y} \left[\frac{C_{00}^{\gamma}(x, y, z, t)}{P^\gamma(x, y, z, t)} \frac{\partial C_{10}(x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[\frac{C_{00}^{\gamma}(x, y, z, t)}{P^\gamma(x, y, z, t)} \frac{\partial C_{10}(x, y, z, t)}{\partial z} \right] \right\} + \left\{ \frac{\partial}{\partial x} \left[g_L(x, y, z, T) \times \right. \right. \\
 & \quad \left. \left. \times \frac{\partial C_{01}(x, y, z, t)}{\partial x} \right] + \frac{\partial}{\partial y} \left[g_L(x, y, z, T) \frac{\partial C_{01}(x, y, z, t)}{\partial y} \right] + \frac{\partial}{\partial z} \left[g_L(x, y, z, T) \frac{\partial C_{01}(x, y, z, t)}{\partial z} \right] \right\} D_{0L}.
 \end{aligned}$$

Solutions of equations for functions $C_{ij}(x, y, z, t)$ ($i \geq 0, j \geq 0$) with account appropriate conditions takes the form

$$\begin{aligned}
 C_{00}(x, y, z, t) &= \frac{1}{L_x L_y L_z} + \frac{2}{L_x L_y L_z} \sum_{n=1}^{\infty} F_{nc} c_n(x) c_n(y) c_n(z) e_{nc}(t), \\
 \text{where } e_{nc}(t) &= \exp \left[-\pi^2 n^2 D_{0c} t \left(\frac{1}{L_x^2} + \frac{1}{L_y^2} + \frac{1}{L_z^2} \right) \right], \quad F_{nc} = \int_0^{L_x} c_n(x) \int_0^{L_y} c_n(y) \int_0^{L_z} c_n(z) f_c(x, y, z) d z d y d x; \\
 C_{i0}(x, y, z, t) &= -\frac{2\pi}{L_x^2 L_y L_z} \sum_{n=1}^{\infty} F_{nc} c_n(x) c_n(y) c_n(z) e_{nc}(t) \int_0^{L_x} e_{nc}(-\tau) \int_0^{L_y} s_n(u) \int_0^{L_z} c_n(v) \int_0^{L_z} c_n(w) g_L(u, v, w, T) \times \\
 & \times \frac{\partial C_{i-10}(u, v, w, \tau)}{\partial u} d w d v d u d \tau - \frac{2\pi}{L_x L_y^2 L_z} \sum_{n=1}^{\infty} n F_{nc} c_n(x) c_n(y) c_n(z) e_{nc}(t) \int_0^{L_x} e_{nc}(-\tau) \int_0^{L_y} c_n(u) \int_0^{L_y} s_n(v) \times \\
 & \times \int_0^{L_z} c_n(w) g_L(u, v, w, T) \frac{\partial C_{i-10}(u, v, w, \tau)}{\partial v} d w d v d u d \tau - \frac{2\pi}{L_x L_y L_z^2} \sum_{n=1}^{\infty} c_n(x) c_n(y) c_n(z) e_{nc}(t) \int_0^{L_x} e_{nc}(-\tau) \times \\
 & \times n F_{nc} \int_0^{L_y} c_n(u) \int_0^{L_y} c_n(v) \int_0^{L_z} s_n(w) g_L(u, v, w, T) \frac{\partial C_{i-10}(u, v, w, \tau)}{\partial w} d w d v d u d \tau, \quad i \geq 1; \\
 C_{01}(x, y, z, t) &= -\frac{2\pi}{L_x^2 L_y L_z} \sum_{n=1}^{\infty} n F_{nc} c_n(x) c_n(y) c_n(z) e_{nc}(t) \int_0^{L_x} e_{nc}(-\tau) \int_0^{L_y} s_n(u) \int_0^{L_z} c_n(v) \int_0^{L_z} c_n(w) \frac{C_{00}^{\gamma}(u, v, w, \tau)}{P^\gamma(u, v, w, T)} \times \\
 & \times c_n(w) \frac{\partial C_{00}(u, v, w, \tau)}{\partial u} d w d v d u d \tau - \frac{2\pi}{L_x L_y^2 L_z} \sum_{n=1}^{\infty} n F_{nc} c_n(x) c_n(y) c_n(z) e_{nc}(t) \int_0^{L_x} e_{nc}(-\tau) \int_0^{L_y} c_n(u) \times \\
 & \times \int_0^{L_y} s_n(v) \int_0^{L_z} c_n(w) \frac{C_{00}^{\gamma}(u, v, w, \tau)}{P^\gamma(u, v, w, T)} \frac{\partial C_{00}(u, v, w, \tau)}{\partial v} d w d v d u d \tau - \frac{2\pi}{L_x L_y L_z^2} \sum_{n=1}^{\infty} n F_{nc} c_n(x) c_n(y) c_n(z) \times \\
 & \times e_{nc}(t) \int_0^{L_x} e_{nc}(-\tau) \int_0^{L_y} c_n(u) \int_0^{L_y} c_n(v) \int_0^{L_z} s_n(w) \frac{C_{00}^{\gamma}(u, v, w, \tau)}{P^\gamma(u, v, w, T)} \frac{\partial C_{00}(u, v, w, \tau)}{\partial w} d w d v d u d \tau;
 \end{aligned}$$

$$\begin{aligned}
 C_{02}(x, y, z, t) = & -\frac{2\pi}{L_x^2 L_y L_z} \sum_{n=1}^{\infty} n F_{nc} c_n(x) c_n(y) c_n(z) e_{nc}(t) \int_0^{L_x} e_{nc}(-\tau) \int_0^{L_y} s_n(u) \int_0^{L_z} c_n(v) \int_0^{L_y} c_n(w) \frac{C_{00}^{\gamma-1}(u, v, w, \tau)}{P^\gamma(u, v, w, T)} \times \\
 & \times \frac{\partial C_{00}(u, v, w, \tau)}{\partial u} dwdvdud\tau - \frac{2\pi}{L_x L_y^2 L_z} \sum_{n=1}^{\infty} n F_{nc} c_n(x) c_n(y) c_n(z) e_{nc}(t) \int_0^{L_x} e_{nc}(-\tau) \int_0^{L_y} s_n(u) \int_0^{L_z} c_n(v) \times \\
 & \times \int_0^{L_z} c_n(w) \frac{C_{00}^{\gamma-1}(u, v, w, \tau)}{P^\gamma(u, v, w, T)} \frac{\partial C_{00}(u, v, w, \tau)}{\partial v} dwdvdud\tau - \frac{2\pi}{L_x L_y L_z^2} \sum_{n=1}^{\infty} n F_{nc} c_n(x) c_n(y) c_n(z) e_{nc}(t) \times \\
 & \times \int_0^{L_x} e_{nc}(-\tau) \int_0^{L_y} c_n(u) \int_0^{L_z} c_n(v) \int_0^{L_y} s_n(w) \frac{C_{00}^{\gamma-1}(u, v, w, \tau)}{P^\gamma(u, v, w, T)} \frac{\partial C_{00}(u, v, w, \tau)}{\partial w} dwdvdud\tau - \frac{2\pi}{L_x^2 L_y L_z} \sum_{n=1}^{\infty} n c_n(x) \times \\
 & \times F_{nc} c_n(y) c_n(z) e_{nc}(t) \int_0^{L_x} e_{nc}(-\tau) \int_0^{L_y} s_n(u) \int_0^{L_z} c_n(v) \int_0^{L_y} c_n(w) \frac{C_{00}^{\gamma}(u, v, w, \tau)}{P^\gamma(u, v, w, T)} \frac{\partial C_{01}(u, v, w, \tau)}{\partial u} dwdvdud\tau - \\
 & - \frac{2\pi}{L_x L_y^2 L_z} \sum_{n=1}^{\infty} n F_{nc} c_n(x) c_n(y) c_n(z) e_{nc}(t) \int_0^{L_x} e_{nc}(-\tau) \int_0^{L_y} s_n(u) \int_0^{L_z} c_n(v) \int_0^{L_y} s_n(w) \frac{C_{00}^{\gamma}(u, v, w, \tau)}{P^\gamma(u, v, w, T)} \frac{\partial C_{01}(u, v, w, \tau)}{\partial v} \times \\
 & \times c_n(w) dwdvdud\tau - \frac{2\pi}{L_x L_y L_z^2} \sum_{n=1}^{\infty} n F_{nc} c_n(x) c_n(y) c_n(z) e_{nc}(t) \int_0^{L_x} e_{nc}(-\tau) \int_0^{L_y} c_n(u) \int_0^{L_z} c_n(v) \int_0^{L_y} s_n(w) \times \\
 & \times \frac{C_{00}^{\gamma}(u, v, w, \tau)}{P^\gamma(u, v, w, T)} \frac{\partial C_{01}(u, v, w, \tau)}{\partial w} dwdvdud\tau; \\
 C_{11}(x, y, z, t) = & -\frac{2\pi}{L_x^2 L_y L_z} \sum_{n=1}^{\infty} n F_{nc} c_n(x) c_n(y) c_n(z) e_{nc}(t) \int_0^{L_x} e_{nc}(-\tau) \int_0^{L_y} s_n(u) \int_0^{L_z} c_n(v) \int_0^{L_y} c_n(w) g_L(u, v, w, T) \times \\
 & \times \frac{\partial C_{01}(u, v, w, \tau)}{\partial u} dwdvdud\tau - \frac{2\pi}{L_x L_y^2 L_z} \sum_{n=1}^{\infty} c_n(x) c_n(y) c_n(z) e_{nc}(t) \int_0^{L_x} e_{nc}(-\tau) \int_0^{L_y} c_n(u) \int_0^{L_z} c_n(v) \int_0^{L_y} c_n(w) \times \\
 & \times n F_{nc} g_L(u, v, w, T) \frac{\partial C_{01}(u, v, w, \tau)}{\partial v} dwdvdud\tau - \frac{2\pi}{L_x L_y L_z^2} \sum_{n=1}^{\infty} c_n(x) c_n(y) c_n(z) e_{nc}(t) \int_0^{L_x} e_{nc}(-\tau) \times \\
 & \times n F_{nc} \int_0^{L_x} c_n(u) \int_0^{L_y} c_n(v) \int_0^{L_z} s_n(w) g_L(u, v, w, T) \frac{\partial C_{01}(u, v, w, \tau)}{\partial w} dwdvdud\tau - \frac{2\pi}{L_x^2 L_y L_z} \sum_{n=1}^{\infty} n F_{nc} c_n(x) \times \\
 & \times c_n(y) c_n(z) e_{nc}(t) \int_0^{L_x} e_{nc}(-\tau) \int_0^{L_y} s_n(u) \int_0^{L_z} c_n(v) \int_0^{L_y} c_n(w) \frac{C_{00}^{\gamma}(u, v, w, \tau)}{P^\gamma(u, v, w, T)} \frac{\partial C_{10}(u, v, w, \tau)}{\partial u} dwdvdud\tau - \\
 & - \frac{2\pi}{L_x L_y^2 L_z} \sum_{n=1}^{\infty} n c_n(x) \int_0^{L_x} e_{nc}(-\tau) \int_0^{L_y} c_n(u) \int_0^{L_z} s_n(v) \int_0^{L_y} c_n(w) \frac{C_{00}^{\gamma}(u, v, w, \tau)}{P^\gamma(u, v, w, T)} \frac{\partial C_{10}(u, v, w, \tau)}{\partial v} dwdvdud\tau \times \\
 & \times F_{nc} c_n(y) c_n(z) e_{nc}(t) - \frac{2\pi}{L_x L_y L_z^2} \sum_{n=1}^{\infty} n F_{nc} c_n(x) c_n(y) c_n(z) e_{nc}(t) \int_0^{L_x} e_{nc}(-\tau) \int_0^{L_y} c_n(u) \int_0^{L_z} c_n(v) \int_0^{L_y} s_n(w) \times \\
 & \times \frac{C_{00}^{\gamma}(u, v, w, \tau)}{P^\gamma(u, v, w, T)} \frac{\partial C_{10}(u, v, w, \tau)}{\partial w} dwdvdud\tau - \frac{2\pi}{L_x^2 L_y L_z} \sum_{n=1}^{\infty} n F_{nc} c_n(x) c_n(y) c_n(z) e_{nc}(t) \int_0^{L_x} e_{nc}(-\tau) \times \\
 & \times \int_0^{L_x} s_n(u) \int_0^{L_y} c_n(v) \int_0^{L_z} c_n(w) \frac{C_{00}^{\gamma-1}(u, v, w, \tau)}{P^\gamma(u, v, w, T)} \frac{\partial C_{00}(u, v, w, \tau)}{\partial u} dwdvdud\tau - \frac{2\pi}{L_x L_y^2 L_z} \sum_{n=1}^{\infty} n F_{nc} c_n(x) \times \\
 & \times c_n(y) c_n(z) e_{nc}(t) \int_0^{L_x} e_{nc}(-\tau) \int_0^{L_y} c_n(u) \int_0^{L_z} s_n(v) \int_0^{L_y} c_n(w) \frac{C_{00}^{\gamma-1}(u, v, w, \tau)}{P^\gamma(u, v, w, T)} \frac{\partial C_{00}(u, v, w, \tau)}{\partial v} dwdvdud\tau - \\
 & - \frac{2\pi}{L_x L_y L_z^2} \sum_{n=1}^{\infty} n \int_0^{L_x} e_{nc}(-\tau) \int_0^{L_y} c_n(u) \int_0^{L_z} c_n(v) \int_0^{L_y} s_n(w) \frac{C_{00}^{\gamma-1}(u, v, w, \tau)}{P^\gamma(u, v, w, T)} \frac{\partial C_{00}(u, v, w, \tau)}{\partial w} dwdvdud\tau \times \\
 & \times F_{nc} c_n(x) c_n(y) c_n(z) e_{nc}(t).
 \end{aligned}$$

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