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On increasing the homogeneity of the properties of epitaxial layers grown from the gas phase, taking into account natural convection and changes in the rate of chemical interaction between materials

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Abstract. In this paper, using the recently introduced analytical approach for the analysis of mass and heat transfer during film growth in reactors for epitaxy from the gas phase, these processes are analyzed taking into account natural convection and the possibility of changing the rate of chemical interaction between reagents. As a result of the analysis, the conditions under which the homogeneity of the grown epitaxial layers increases with a change in the values of the parameters of the growth process are formulated.

Keywords: growth; heat transfer; material fabrication; mathematical modelling

1. Introduction

At present, different heterostructures are widely used for manufacture solid-state electronics devices. The most common methods of growing heterostructures are epitaxy from the gas and liquid phases, magnetron sputtering, and molecular beam epitaxy. A large number of experimental studies are devoted to the manufacturing and using of heterostructures due to their wide using (see, for example, Stepanenko 1980, Gusev and Gusev 1991, Lachin and Savelov 2001, Vorob'ev *et al*. 2003, Sorokin *et al*. 2008, Lundin *et al*. 2009, Hosseini and Sarvi 2015, Li *et al*. 2006, Chakraborty *et al*. 2004, Taguchia *et al*. 2016, *Mitsuhara et al*. 1998). At the same time, a relatively small number of works are devoted to predicting epitaxy processes (see, for example, Talalaev *et al*. 2001). The main aim of this work is to analyze changing of properties of the grown epitaxial layers with a changing of the values of the parameters of the growth process, taking into account natural convection.

In this paper, we consider a vertical reactor for epitaxy from the gas phase (see Fig. 1). This reactor consists of a external casing, keeper of substrate with a substrate and a spiral around the shell in the region of the formation of the epitaxial layer in order to provide induction heating to activate chemical reactions that take place during the decomposition of the reactants and the growth of the epitaxial layer. A gaseous mixture of reactants is fed to the inlet of the reaction chamber together with a gas- carrier. The main aim of this work is to analyze the changes in the properties of the grown

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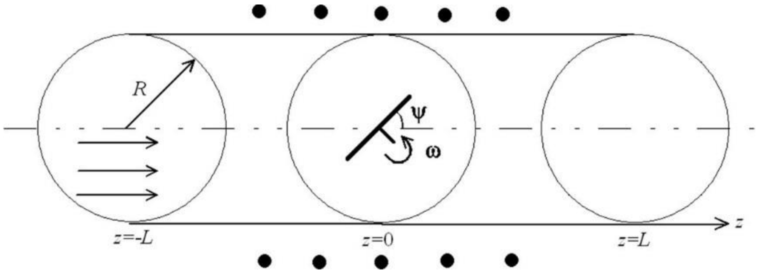
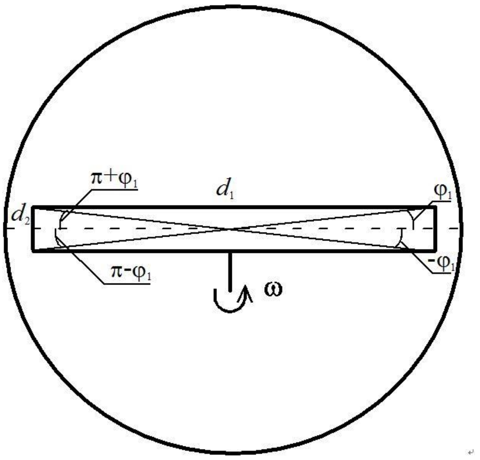


(a) Structure of reactor for gas phase epitaxy with sloping keeper of substrate



(b) View from side of keeper of substrate and approximation of the keeper by sloping lines with angle of sloping φ_1

Fig. 1 Construction of reactor for gas phase epitaxy: side view (a) and in front (b)

epitaxial layers with changes in the values of the parameters of the growth process, taking into account natural convection.

2. Method of solution

To solve the considered aims, we determine the spatio-temporal distribution of the temperature. We determined the considered temperature by solution of the following boundary value problem (see, for example, Carslaw and Jaeger 1964)

$$\begin{aligned} c\frac{\partial T(r,\phi,z,t)}{\partial t} &= div\{\lambda \cdot grad[T(r,\phi,z,t)] - [\vec{v}(r,\phi,z,t) - \vec{\bar{v}}(r,\phi,z,t)] \\ &\quad \cdot c(T) \cdot T(r,\phi,z,t) \cdot C_\Sigma(r,\phi,z,t)\} + p(r,\phi,z,t) \end{aligned} \tag{1}$$

where $\vec{v}$ is the speed of mixture of gases; c is the heat capacity of the system; $T(r, \varphi, z, t)$ is the space-time temperature distribution; $p(r, \varphi, z, t)$ is the density of the power released in the system substrate-holder; r, φ, z and t are the current cylindrical coordinates and time; $C_\Sigma(r, \varphi, z, t)$ is the spatio-temporal distribution of the concentration of the gas mixture consisting of reactant gases (we will assume that two gases-reagents with concentrations of C_1 (r, φ, z, t) and C_2 (r, φ, z, t) enter the reactor) and the material of the epitaxial layer in the gas phase with a concentration of C_3 (r, φ, z, t); λ is the coefficient of thermal conductivity, the value of which is determined by the ratio: $\lambda = \bar{v}\bar{l}c_v\rho/3$, where $\bar{v}$ is the modulus of the mean-square velocity of the gas molecules, equal to $\bar{v} = \sqrt{2kT/m}$; $\bar{l}$ is the mean free path of gas molecules between collisions, c_v is the heat capacity of the gas at constant volume, ρ is the gas density. The first term of Eq. (1) describes free heat transport in gases, liquids and solids without influence of any factors (additional heating, cooling, ...). The second term describes changing of free heat transport under influence of native and forced convection (forced flow of gas around heated keeper of substrate with substrate). The third term of Eq. (3) describes power of heating of the considered system due to induction.

To solve the Eq. (1) it is necessary to take into account the flow of the gas mixture and its concentration. We shall determine the required values by solving the Navier-Stokes equation (i.e. the Eq. (2)) and the second Fick's laws (i.e., the Eq. (3)), respectively. In this case, we assume that the radius of the substrate holder R substantially exceeds the thickness of the diffusion and boundary layers, and we assume that the flow of gas is laminar. In this case, these equations are written in the form

$$\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla)\vec{v} = -\nabla\left(\frac{P}{\rho}\right) + \nu \Delta \vec{v}, \tag{2}$$

$$\begin{aligned}\frac{\partial C_1(r,\phi,z,t)}{\partial t} = {} & div\left\{D_1 \cdot grad\left[C_1(r,\phi,z,t)\right] - \left[\vec{v}(r,\phi,z,t) - \vec{\bar{v}}\right] \cdot C_1(r,\phi,z,t)\right\} \\ & -k_1(r,\phi,z,t) \cdot C_1(r,\phi,z,t),\end{aligned} \tag{3a}$$

$$\begin{aligned}\frac{\partial C_2(r,\phi,z,t)}{\partial t} = {} & div\left\{D_2 \cdot grad\left[C_2(r,\phi,z,t)\right] - \left[\vec{v}(r,\phi,z,t) - \vec{\bar{v}}\right] \cdot C_2(r,\phi,z,t)\right\} \\ & - k_2(r,\phi,z,t) \cdot C_2(r,\phi,z,t),\end{aligned} \tag{3b}$$

$$\begin{aligned}\frac{\partial C_3(r,\phi,z,t)}{\partial t} = {} & div\left\{D_3 \cdot grad\left[C_3(r,\phi,z,t)\right] - \left[\vec{v}(r,\phi,z,t) - \vec{\bar{v}}\right] \cdot C_3(r,\phi,z,t)\right\} \\ & + k_3(r,\phi,z,t) \cdot C_3(r,\phi,z,t).\end{aligned} \tag{3c}$$

Here D_i are the diffusion coefficients of the gases-reagents (as an example, this can be trimethylgallium $(CH_3)_3Ga$ and arsenic hydride AsH_3) and the resulting gas, which will be obtained after reaction of the reactant gases under consideration as an epitaxial layer in the gas phase (in the framework of the considered example, it is $GaAs$) in the carrier gas (as an example, it can be hydrogen); P is the gas pressure in the reactor; ν is the kinematic viscosity. The Eq. (2) describes transport of gases. The left side of the equation describes changing of speed of gases in time. The right side of the Eq. (2) describes external influence on speed of gases by changing of external pressure (the first term in the right side) and dissipation of gas flow due to viscosity of the considered gas (the second term in the right side). The first terms of the right sides of Eq. (3) describe thermal diffusion of reagents and material of epitaxial layer. The second terms of the right sides of Eq. (3) describe losing of materials due to convection. The third terms of the right sides of Eq. (3) describe losing of reagents and generation of material of epitaxial layer due to reaction.

Now we consider the boundary and initial conditions with account the limiting flow regime, when all the molecules of the deposited substance approaching the disk are deposited on the substrate, homogeneity and one-dimensionality of the flow at the entrance to the reaction zone. In the considered system, mass and heat transfer processes proceed in a cylindrical reactor, which makes it appropriate to use a cylindrical coordinate system. At the same time, the substrate holder with the substrate breaks the cylindrical symmetry of the system. We shall consider the substrate holder approximately rectangular along the z axis with those indicated in Fig. 1(b) in size. To go to a single (cylindrical) coordinate system, we approximate the natural obstacle for gases in the reactor (substrate holder) by two inclined straight lines passing through the center of the substrate holder (see Fig. 1(b)). In this case, due to the usual relationship between the size of the substrate holder $d_2 << d_1$, the angle of inclination of the straight lines φ_1 is small. The boundary and initial conditions in the considered system with the considered approximations could be written as

$$\begin{gathered}
C_1(r,\varphi,-L,t)=C_2(r,\varphi,-L,t)=C_0,\ C_3(r,\varphi,-L,t)=0;\\
C_i(r,-\varphi_1,z,t)=C_i(r,\varphi_1,z,t)=C_i(r,\pi-\varphi_1,z,t)=C_i(r,\pi+\varphi_1,z,t);\\
C_1(r,\varphi,z,0)=C_2(r,\varphi,z,0)=C_0\delta(z+L),\ C_3(r,\varphi,z,0)=0;\\
C_i(0,\varphi,z,t)\neq\infty;\ C_i(r,\phi,z,t)\big|_S=0;\\
T(r,-\varphi_1,z,t)=T(r,\varphi_1,z,t)=T(r,\pi-\varphi_1,z,t)=T(r,\pi+\varphi_1,z,t);\\
-\lambda\frac{\partial T(r,\phi,z,t)}{\partial r}\bigg|_S=\sigma T^4(R,\phi,z,t);\ \frac{\partial T(r,\phi,z,t)}{\partial\phi}\bigg|_{\phi=0}=\frac{\partial T(r,\phi,z,t)}{\partial\phi}\bigg|_{\phi=2\pi};\\
T(r,\varphi,z,0)=T_r;\ T(0,\varphi,z,t)\neq\infty;\ \frac{\partial C_i(r,\phi,z,t)}{\partial r}\bigg|_{r=R}=0;\\
-\lambda\frac{\partial T(r,\phi,z,t)}{\partial z}\bigg|_S=\sigma T^4(r,\phi,-L,t);\ \frac{\partial v_r(r,\phi,z,t)}{\partial r}\bigg|_{r=0}=0;\\
v_r(r,-\varphi_1,z,t)=v_r(r,\varphi_1,z,t)=v_r(r,\pi-\varphi_1,z,t)=v_r(r,\pi+\varphi_1,z,t);\\
\frac{\partial v_r(r,\phi,z,t)}{\partial r}\bigg|_{r=R}=0;\ v_\varphi(r,-\varphi_1,z,t)=v_\varphi(r,\varphi_1,z,t)=v_\varphi(r,\pi-\varphi_1,z,t)=v_\varphi(r,\pi+\varphi_1,z,t);\\
v_z(r,-\varphi_1,z,t)=v_z(r,\varphi_1,z,t)=v_z(r,\pi-\varphi_1,z,t)=v_z(r,\pi+\varphi_1,z,t);\ v_r(r,\varphi,-L,t)=0;\\
v_r(r,\varphi,L,t)=0;\ v_r(0,\varphi,z,t)\neq\infty;\ v_z(r,\varphi,-L,t)=V_0;\\
v_z(r\pm d_2/2,\varphi,z\in[-d_2/2,d_2/2],0)=\omega\cdot z\cdot\cos\psi\,tg(\varphi_1);\ v_\varphi(r,\varphi,L,t)=0;\ v_\varphi(0,\varphi,z,t)\neq\infty;\\
v_z(r,\varphi,0,t)=0;\ v_z(r,\varphi,L,t)=V_0,\ v_z(r,\varphi,L,t)=V_0,\ v_z(0,\varphi,z,t)\neq\infty;\ v_r(r,\varphi,z,0)=0;\\
v_\varphi(r,\varphi,z,0)=0;\ v_\varphi(r,\varphi,0,t)=\omega r,
\end{gathered}\tag{4}$$

where $\sigma=5{,}67\cdot10^{-8}\ \mathrm{W}\cdot m^{-2}\cdot K^{-4}$, T_r is the room temperature, ω is the rotation frequency of the substrate.

We consider cylindrical reactor for gas phase epitaxy. In a cylindrical coordinate system, the equations for the velocity projections have the following form

$$\begin{gathered}
\frac{\partial v_r}{\partial t}=\nu\left\{\frac{1}{r}\frac{\partial}{\partial r}\left[r\frac{\partial v_r(r,\phi,z,t)}{\partial r}\right]+\frac{1}{r^2}\frac{\partial^2 v_r(r,\phi,z,t)}{\partial\phi^2}+\frac{\partial^2 v_r(r,\phi,z,t)}{\partial z^2}\right\}\\
-v_r\frac{\partial v_r}{\partial r}-\frac{v_\phi}{r}\frac{\partial v_\phi}{\partial\phi}-v_z\frac{\partial v_z}{\partial z}-\frac{\partial}{\partial r}\left(\frac{P}{\rho}\right)
\end{gathered}\tag{5a}$$

$$\begin{gathered}
\frac{\partial v_r}{\partial t}=\nu\left\{\frac{1}{r}\frac{\partial}{\partial r}\left[r\frac{\partial v_\phi(r,\phi,z,t)}{\partial r}\right]+\frac{1}{r^2}\frac{\partial^2 v_\phi(r,\phi,z,t)}{\partial\phi^2}+\frac{\partial^2 v_\phi(r,\phi,z,t)}{\partial z^2}\right\}\\
-v_r\frac{\partial v_r}{\partial r}-\frac{v_\phi}{r}\frac{\partial v_\phi}{\partial\phi}-v_z\frac{\partial v_z}{\partial z}-\frac{1}{r}\frac{\partial}{\partial\phi}\left(\frac{P}{\rho}\right)
\end{gathered}\tag{5b}$$

$$\frac{\partial v_z}{\partial t}=\nu\left\{\frac{1}{r}\frac{\partial}{\partial r}\left[r\frac{\partial v_z(r,\phi,z,t)}{\partial r}\right]+\frac{1}{r^2}\frac{\partial^2 v_z(r,\phi,z,t)}{\partial \phi^2}+\frac{\partial^2 v_z(r,\phi,z,t)}{\partial z^2}\right\}$$
$$-v_r\frac{\partial v_r}{\partial r}-\frac{v_\phi}{r}\frac{\partial v_\phi}{\partial \phi}-v_z\frac{\partial v_z}{\partial z}-\frac{\partial}{\partial z}\left(\frac{P}{\rho}\right). \qquad (5c)$$

Let us determine solution of this system of equations using the method of averaging functional corrections (Sokolov 1955, Pankratov and Bulaeva 2013a, 2016a, b, Pankratov 2017a, b). In the framework of this method, to determine the first approximation of the projections of the gas flow rate of the gas mixture, we replace them with the yet unknown mean values $v_r \to \alpha_{1r}$, $v_\varphi \to \alpha_{1\varphi}$, $v_z \to \alpha_{1z}$ in the right side of the equations of system (5). After such a substitution, we obtain the equations for the first approximations of the desired components in the following form

$$\frac{\partial v_{1r}}{\partial t}=-\frac{\partial}{\partial r}\left(\frac{P}{\rho}\right),\qquad \frac{\partial v_{1\phi}}{\partial t}=-\frac{1}{r}\frac{\partial}{\partial \phi}\left(\frac{P}{\rho}\right),\qquad \frac{\partial v_{1z}}{\partial t}=-\frac{\partial}{\partial z}\left(\frac{P}{\rho}\right). \qquad (6)$$

Solutions of these equations could be written as

$$v_{1r}=-\frac{\partial}{\partial r}\int_0^t\frac{P}{\rho}d\tau,\qquad v_{1\phi}=-\frac{1}{r}\frac{\partial}{\partial \phi}\int_0^t\frac{P}{\rho}d\tau,\qquad v_{1z}=-\frac{\partial}{\partial z}\int_0^t\frac{P}{\rho}d\tau. \qquad (7)$$

The second-order approximations of the velocity projections can be obtained by replacing the desired projections in the right-hand side of the equations of system (5) by the sums $v_r \to \alpha_{2r} + v_{1r}$, $v_\varphi \to \alpha_{2\varphi} + v_{1\varphi}$, $v_z \to \alpha_{2z} + v_{1z}$. The equations for these projections have the form

$$\frac{\partial v_{2r}}{\partial t}=\nu\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_{1r}}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 v_{1r}}{\partial \phi^2}+\frac{\partial^2 v_{1r}}{\partial z^2}\right]-\frac{\partial}{\partial r}\left(\frac{P}{\rho}\right)-(\alpha_{2r}+v_{1r})\frac{\partial v_{1r}}{\partial r}$$
$$-\frac{(\alpha_{2\phi}+v_{1\phi})}{r}\frac{\partial v_{1r}}{\partial \phi}-(\alpha_{2z}+v_{1z})\frac{\partial v_{1r}}{\partial z}, \qquad (8a)$$

$$\frac{\partial v_{2\phi}}{\partial t}=\nu\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_{1\phi}}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 v_{1\phi}}{\partial \phi^2}+\frac{\partial^2 v_{1\phi}}{\partial z^2}\right]-\frac{1}{r}\frac{\partial}{\partial \phi}\left(\frac{P}{\rho}\right)-(\alpha_{2r}+v_{1r})\frac{\partial v_{1\phi}}{\partial r}$$
$$-\frac{(\alpha_{2\phi}+v_{1\phi})}{r}\frac{\partial v_{1\phi}}{\partial \phi}-(\alpha_{2z}+v_{1z})\frac{\partial v_{1\phi}}{\partial z}, \qquad (8b)$$

$$\frac{\partial v_{2z}}{\partial t}=\nu\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_{1z}}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 v_{1z}}{\partial \phi^2}+\frac{\partial^2 v_{1z}}{\partial z^2}\right]-\frac{\partial}{\partial z}\left(\frac{P}{\rho}\right)-(\alpha_{2r}+v_{1r})\frac{\partial v_{1z}}{\partial r}$$
$$-\frac{(\alpha_{2\phi}+v_{1\phi})}{r}\frac{\partial v_{1z}}{\partial \phi}-(\alpha_{2z}+v_{1z})\frac{\partial v_{1z}}{\partial z}. \qquad (8c)$$

Integration of these equations leads to the following result

$$v_{2r}=\nu\int_0^t\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_{1r}}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 v_{1r}}{\partial \phi^2}+\frac{\partial^2 v_{1r}}{\partial z^2}\right]d\tau-\frac{\partial}{\partial r}\left(\int_0^t\frac{P}{\rho}d\tau\right) \qquad (8d)$$

$$-\int_0^t (\alpha_{2r}+v_{1r})\frac{\partial v_{1r}}{\partial r}d\tau-\int_0^t \frac{(\alpha_{2\phi}+v_{1\phi})}{r}\frac{\partial v_{1r}}{\partial \phi}d\tau-\int_0^t (\alpha_{2z}+v_{1z})\frac{\partial v_{1r}}{\partial z}d\tau, \tag{8d}$$

$$\begin{aligned} v_{2\phi}=\nu\int_0^t\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_{1\phi}}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 v_{1\phi}}{\partial \phi^2}+\frac{\partial^2 v_{1\phi}}{\partial z^2}\right]d\tau-\frac{1}{r}\frac{\partial}{\partial \phi}\left(\int_0^t\frac{P}{\rho}d\tau\right)\\ -\int_0^t (\alpha_{2r}+v_{1r})\frac{\partial v_{1\phi}}{\partial r}d\tau-\int_0^t \frac{(\alpha_{2\phi}+v_{1\phi})}{r}\frac{\partial v_{1\phi}}{\partial \phi}d\tau-\int_0^t (\alpha_{2z}+v_{1z})\frac{\partial v_{1\phi}}{\partial z}d\tau \end{aligned} \tag{8e}$$

$$\begin{aligned} v_{2z}=V_0+\nu\int_0^t\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_{1z}}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 v_{1z}}{\partial \phi^2}+\frac{\partial^2 v_{1z}}{\partial z^2}\right]d\tau-\frac{\partial}{\partial z}\left(\int_0^t\frac{P}{\rho}d\tau\right)\\ -\int_0^t (\alpha_{2r}+v_{1r})\frac{\partial v_{1z}}{\partial r}d\tau-\int_0^t \frac{(\alpha_{2\phi}+v_{1\phi})}{r}\frac{\partial v_{1z}}{\partial \phi}d\tau-\int_0^t (\alpha_{2z}+v_{1z})\frac{\partial v_{1z}}{\partial z}d\tau. \end{aligned} \tag{8f}$$

Average values α_{2r}, $\alpha_{2\varphi}$, α_{2z} have been determine by the following relations

$$\begin{aligned} \alpha_{2r}&=\frac{1}{\pi\Theta R^2 L}\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^L (v_{2r}-v_{1r})dzd\phi drdt\,,\\ \alpha_{2\phi}&=\frac{1}{\pi\Theta R^2 L}\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^L (v_{2\phi}-v_{1\phi})dzd\phi drdt\,,\\ \alpha_{2z}&=\frac{1}{\pi\Theta R^2 L}\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^L (v_{2z}-v_{1z})dzd\phi drdt. \end{aligned} \tag{9}$$

where Θ is the continuance of the flow of the mixture of gases. Substituting the first two approximations of the velocity projections into relations (9) allows us to obtain a system of equations for the required average values.

$$\begin{cases} A_1\alpha_{2r}+B_1\alpha_{2\phi}+C_1\alpha_{2z}=D_1\\ A_2\alpha_{2r}+B_2\alpha_{2\phi}+C_2\alpha_{2z}=D_2\\ A_3\alpha_{2r}+B_3\alpha_{2\phi}+C_3\alpha_{2z}=D_3 \end{cases} \tag{10}$$

where $A_1=1+\int_0^\Theta(\Theta-t)\int_0^R r\int_0^{2\pi}\int_{-L}^L\frac{\partial v_{1r}}{\partial r}dzd\phi drdt\,,$

$$B_1=\int_0^\Theta(\Theta-t)\int_0^R\int_0^{2\pi}\int_{-L}^L\frac{\partial v_{1r}}{\partial \phi}dzd\phi drdt,$$

$$C_1=C_2=\frac{\pi}{2}\Theta^2R^2V_0,$$

$$\begin{aligned} D_1=\nu\int_0^\Theta(\Theta-t)\int_0^R r\int_0^{2\pi}\int_{-L}^L\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_{1r}}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2 v_{1r}}{\partial \phi^2}+\frac{\partial^2 v_{1r}}{\partial z^2}\right]dzd\phi drdt\\ -\int_0^\Theta(\Theta-t)\int_0^R r\int_0^{2\pi}\int_{-L}^L v_{1r}\frac{\partial v_{1r}}{\partial r}dzd\phi drdt-\frac{\pi}{8}\Theta^2R^2V_0^2\\ -\int_0^\Theta(\Theta-t)\int_0^R\int_0^{2\pi}\int_{-L}^L v_{1\phi}\frac{\partial v_{1r}}{\partial \phi}dzd\phi drdt\,, \end{aligned}$$

$$
\begin{aligned}
A_2 &= \int_0^{\Theta} (\Theta - t) \int_0^R r \int_0^{2\pi} \int_{-L}^{L} \frac{\partial v_{1r}}{\partial r} dz d\phi dr dt\,,\\
B_2 &= 1 + \int_0^{\Theta} (\Theta - t) \times \int_0^R \int_0^{2\pi} \int_{-L}^{L} \frac{\partial v_{1r}}{\partial \phi} dz d\phi dr dt\,,\\
D_2 &= \nu \int_0^{\Theta} (\Theta - t) \int_0^R r \int_0^{2\pi} \int_{-L}^{L} \left[\frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial v_{1\phi}}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 v_{1\phi}}{\partial \phi^2} + \frac{\partial^2 v_{1\phi}}{\partial z^2}\right] dz d\phi dr dt\\
&\quad - \int_0^{\Theta} (\Theta - t) \times \int_0^R r \int_0^{2\pi} \int_{-L}^{L} v_{1r} \frac{\partial v_{1r}}{\partial r} dz d\phi dr dt\\
&\quad - \int_0^{\Theta} (\Theta - t) \int_0^R \int_0^{2\pi} \int_{-L}^{L} v_{1\phi} \frac{\partial v_{1r}}{\partial \phi} dz d\phi dr dt - \frac{\pi}{8}\Theta^2 R^2 V_0^2,\\
A_3 &= \int_0^{\Theta} (\Theta - t) \int_0^R \int_0^{2\pi} \int_{-L}^{L} \frac{\partial v_{1z}}{\partial r} dz d\phi \times r dr dt,\\
B_3 &= \int_0^{\Theta} (\Theta - t) \int_0^R r \int_0^{2\pi} \int_{-L}^{L} \frac{\partial v_{1z}}{\partial \phi} dz d\phi dr dt\,,\\
D_3 &= \int_0^{\Theta} \int_0^R r \int_0^{2\pi} \int_{-L}^{L} \left[\frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial v_{1z}}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 v_{1z}}{\partial \phi^2} + \frac{\partial^2 v_{1z}}{\partial z^2}\right] dz d\phi dr \times \nu(\Theta - t) dt - \frac{\pi}{8}\Theta^2 R^2 V_0^2\\
&\quad - \int_0^{\Theta} \int_0^R r \int_0^{2\pi} \int_{-L}^{L} v_{1r} \frac{\partial v_{1z}}{\partial r} dz d\phi dr dt - \int_0^{\Theta} (\Theta - t) \int_0^R r \int_0^{2\pi} \int_{-L}^{L} v_{1\phi} \frac{\partial v_{1z}}{\partial \phi} dz d\phi dr dt\,,\\
C_3 &= 1 + \frac{\pi}{2} \times \Theta^2 R^2 V_0.
\end{aligned}
$$

Solution of the above system of equations could be determined by standard approaches (see, for example, Korn and Korn 1968) and could be written as

$$
\alpha_{2r} = \Delta_r/\Delta, \qquad \alpha_{2\phi} = \Delta_\phi/\Delta, \qquad \alpha_{2z} = \Delta_z/\Delta, \tag{11}
$$

where $\Delta = A_1(B_2C_3 - B_3C_2) - B_1(A_2C_3 - A_3C_2) + C_1(A_2B_3 - A_3B_2)$, $\Delta_r = D_1(B_2C_3 - B_3C_2) - B_1(D_2C_3 - D_3C_2) + C_1(D_2B_3 - D_3B_2)$, $\Delta_\phi = D_1(B_2C_3 - B_3C_2) - B_1(D_2C_3 - D_3C_2) + C_1 (D_2B_3 - D_3B_2)$, $\Delta_z = A_1(B_2D_3 - B_3D_2) - B_1(A_2D_3 - A_3D_2) + D_1(A_2B_3 - A_3B_2)$.

In this section, we obtained the projections of the flow rate of the mixture of gas-reagents used to form the epitaxial layer and the gas-carrier in the second-order approximation by the method of averaging functional corrections. Usually, the second-order approximation is sufficient to conduct a qualitative analysis of the solution obtained and to conduct some quantitative estimates. Next let us transform Eqs. (1) and (3) in a cylindrical coordinate system

$$
\begin{aligned}
c\frac{\partial T(r,\phi,z,t)}{\partial t} = \lambda \frac{\partial^2 T(r,\phi,z,t)}{\partial r^2} + \lambda \frac{1}{r^2}\frac{\partial^2 T(r,\phi,z,t)}{\partial \phi^2} + \lambda \frac{\partial^2 T(r,\phi,z,t)}{\partial z^2} + p(r,\phi,z,t)&\\
-c \cdot \frac{\partial}{\partial r}\{C_\Sigma(r,\phi,z,t) \cdot [v_r(r,\phi,z,t) - \bar{v}_r(r,\phi,z,t)] \cdot T(r,\phi,z,t)\}&\\
-\frac{c}{r}\frac{\partial}{\partial \phi}\{[v_r(r,\phi,z,t) - \bar{v}_r(r,\phi,z,t)] \cdot C_\Sigma(r,\phi,z,t) \cdot T(r,\phi,z,t)\}&\\
-c \cdot \frac{\partial}{\partial z}\{[v_z(r,\phi,z,t) - \bar{v}_z(r,\phi,z,t)] \cdot C_\Sigma(r,\phi,z,t) \cdot T(r,\phi,z,t)\},&
\end{aligned} \tag{12}
$$

$$\begin{aligned}\frac{\partial C_1(r,\phi,z,t)}{\partial t} &= \frac{1}{r}\frac{\partial}{\partial r}\left[rD_1\frac{\partial C_1(r,\phi,z,t)}{\partial r}\right]+\frac{1}{r^2}\frac{\partial}{\partial \phi}\left[D_1\frac{\partial C_1(r,\phi,z,t)}{\partial \phi}\right]+\frac{\partial}{\partial z}\left[D_1\frac{\partial C_1(r,\phi,z,t)}{\partial z}\right]\\ &-\frac{1}{r}\frac{\partial}{\partial r}\{rC_1(r,\phi,z,t)\cdot[v_r(r,\phi,z,t)-\bar{v}_r(r,\phi,z,t)]\}\\ &-\frac{1}{r}\frac{\partial}{\partial \phi}\left\{rC_1(r,\phi,z,t)\cdot\left[v_\phi(r,\phi,z,t)-\bar{v}_\phi(r,\phi,z,t)\right]\right\}\\ &-\frac{\partial}{\partial z}\{C_1(r,\phi,z,t)\cdot[v_z(r,\phi,z,t)-\bar{v}_z(r,\phi,z,t)]\}\\ &-k_1(r,\phi,z,t)\cdot C_1(r,\phi,z,t),\end{aligned} \tag{13a}$$

$$\begin{aligned}\frac{\partial C_2(r,\phi,z,t)}{\partial t} &= \frac{1}{r}\frac{\partial}{\partial r}\left[rD_2\frac{\partial C_2(r,\phi,z,t)}{\partial r}\right]+\frac{1}{r^2}\frac{\partial}{\partial \phi}\left[D_2\frac{\partial C_2(r,\phi,z,t)}{\partial \phi}\right]+\frac{\partial}{\partial z}\left[D_2\frac{\partial C_2(r,\phi,z,t)}{\partial z}\right]\\ &-\frac{1}{r}\frac{\partial}{\partial r}\{rC_2(r,\phi,z,t)\cdot[v_r(r,\phi,z,t)-\bar{v}_r(r,\phi,z,t)]\}\\ &-\frac{1}{r}\frac{\partial}{\partial \phi}\left\{rC_2(r,\phi,z,t)\cdot\left[v_\phi(r,\phi,z,t)-\bar{v}_\phi(r,\phi,z,t)\right]\right\}\\ &-\frac{\partial}{\partial z}\{C_2(r,\phi,z,t)\cdot[v_z(r,\phi,z,t)-\bar{v}_z(r,\phi,z,t)]\}\\ &-k_2(r,\phi,z,t)\cdot C_2(r,\phi,z,t),\end{aligned} \tag{13b}$$

$$\begin{aligned}\frac{\partial C_3(r,\phi,z,t)}{\partial t} &= \frac{1}{r}\frac{\partial}{\partial r}\left[rD_3\frac{\partial C_3(r,\phi,z,t)}{\partial r}\right]+\frac{1}{r^2}\frac{\partial}{\partial \phi}\left[D_3\frac{\partial C_3(r,\phi,z,t)}{\partial \phi}\right]+\frac{\partial}{\partial z}\left[D_3\frac{\partial C_3(r,\phi,z,t)}{\partial z}\right]\\ &-\frac{1}{r}\frac{\partial}{\partial r}\{rC_3(r,\phi,z,t)\cdot[v_r(r,\phi,z,t)-\bar{v}_r(r,\phi,z,t)]\}\\ &-\frac{1}{r}\frac{\partial}{\partial \phi}\left\{rC_3(r,\phi,z,t)\cdot\left[v_\phi(r,\phi,z,t)-\bar{v}_\phi(r,\phi,z,t)\right]\right\}\\ &-\frac{\partial}{\partial z}\{C_3(r,\phi,z,t)\cdot[v_z(r,\phi,z,t)-\bar{v}_z(r,\phi,z,t)]\}\\ &-k_3(r,\phi,z,t)\cdot C_3(r,\phi,z,t).\end{aligned} \tag{13c}$$

To determine the spatio-temporal distributions of temperature and concentration of the gas mixture, we use the method of averaging functional corrections. To determine the first-order approximations of the unknown functions, we replace them with as yet unknown mean values α_{1T} and α_{i1C} in the right sides of these equations. Using the above algorithm, we obtain the relations for the first approximations of temperature and concentration of a mixture of gases in the following form

$$\begin{aligned}T_1(r,\phi,z,t) &= T_r-\alpha_{1T}\alpha_{1C}\int_0^t\frac{\partial[v_r(r,\phi,z,\tau)-\bar{v}_r(r,\phi,z,\tau)]}{\partial r}d\tau\\ &-\frac{\alpha_{1T}\alpha_{1C}}{r}\int_0^t\frac{\partial\left[v_\phi(r,\phi,z,\tau)-\bar{v}_\phi(r,\phi,z,\tau)\right]}{\partial \phi}d\tau\\ &-\alpha_{1T}\alpha_{1C}\int_0^t\frac{\partial[v_z(r,\phi,z,\tau)-\bar{v}_z(r,\phi,z,\tau)]}{\partial z}d\tau+\int_0^t\frac{p(r,\phi,z,\tau)}{c}d\tau,\end{aligned} \tag{14}$$

$$\begin{aligned} C_{11}(r,\phi,z,t) = {} & -\frac{\alpha_{11C}}{r}\int_0^t \frac{\partial\{r[v_r(r,\phi,z,\tau)-\bar{v}_r(r,\phi,z,\tau)]\}}{\partial r}d\tau - \alpha_{11C}\int_0^t k_1(r,\phi,z,\tau)d\tau \\ & +C_0 - \frac{\alpha_{11C}}{r}\int_0^t \frac{\partial\left[v_\phi(r,\phi,z,\tau)-\bar{v}_\phi(r,\phi,z,\tau)\right]}{\partial\phi}d\tau \\ & -\alpha_{11C}\int_0^t \frac{\partial[v_z(r,\phi,z,\tau)-\bar{v}_z(r,\phi,z,\tau)]}{\partial z}d\tau, \end{aligned} \tag{15a}$$

$$\begin{aligned} C_{21}(r,\phi,z,t) = {} & -\frac{\alpha_{21C}}{r}\int_0^t \frac{\partial\{r[v_r(r,\phi,z,\tau)-\bar{v}_r(r,\phi,z,\tau)]\}}{\partial r}d\tau \\ & +C_0 - \alpha_{21C}\int_0^t k_2(r,\phi,z,\tau)d\tau \\ & -\frac{\alpha_{21C}}{r}\int_0^t \frac{\partial\left[v_\phi(r,\phi,z,\tau)-\bar{v}_\phi(r,\phi,z,\tau)\right]}{\partial\phi}d\tau \\ & -\alpha_{21C}\int_0^t \frac{\partial[v_z(r,\phi,z,\tau)-\bar{v}_z(r,\phi,z,\tau)]}{\partial z}d\tau, \end{aligned} \tag{15b}$$

$$\begin{aligned} C_{31}(r,\phi,z,t) = {} & -\frac{\alpha_{31C}}{r}\int_0^t \frac{\partial\{r[v_r(r,\phi,z,\tau)-\bar{v}_r(r,\phi,z,\tau)]\}}{\partial r}d\tau + \alpha_{31C}\int_0^t k_3(r,\phi,z,\tau)d\tau \\ & -\frac{\alpha_{31C}}{r}\int_0^t \frac{\partial\left[v_\phi(r,\phi,z,\tau)-\bar{v}_\phi(r,\phi,z,\tau)\right]}{\partial\phi}d\tau \\ & -\alpha_{31C}\int_0^t \frac{\partial[v_z(r,\phi,z,\tau)-\bar{v}_z(r,\phi,z,\tau)]}{\partial z}d\tau. \end{aligned} \tag{15c}$$

Now we calculate not yet known average values of the first-order approximations of the considered functions by the following relations

$$\begin{aligned} \alpha_{1T} &= \frac{1}{\pi\Theta R^2 L}\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^L T_1(r,\phi,z,\tau)dzd\phi drdt, \\ \alpha_{i1C} &= \frac{1}{\pi\Theta R^2 L}\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^L C_{i1}(r,\phi,z,\tau)dzd\phi drdt. \end{aligned} \tag{16}$$

Substitution of these first-order approximations of concentrations and temperature into relations (16) leads to the following results

$$\begin{aligned} \alpha_{iC} &= C_0/L\cdot\left\{1+\frac{1}{\pi\Theta RL}\int_0^\Theta(\Theta-t)\int_0^{2\pi}\int_{-L}^L[v_r(R,\phi,z,t)-\bar{v}_r(R,\phi,z,t)]dzd\phi dt+\frac{\Theta V_0}{RL}\right\}, \\ \alpha_{1T} &= \left[T_r+\frac{1}{\pi\Theta R^2 L}\int_0^\Theta(\Theta-t)\int_0^R r\int_0^{2\pi}\int_{-L}^L\frac{p(r,\phi,z,t)}{c}dzd\phi drdt\right] \\ & \quad \Bigg(1+\frac{C_0L^{-2}}{\pi\Theta R}\Bigg\{\int_0^\Theta\int_0^{2\pi}\int_{-L}^L[v_r(R,\phi,z,\tau)-\bar{v}_r(R,\phi,z,\tau)]dzd\phi\times(\Theta-t)dt \\ & \quad +\frac{V_0}{2}-\frac{1}{\pi\Theta R^2}\int_0^\Theta(\Theta-t)\int_0^R\int_0^{2\pi}\int_{-L}^L[v_r(r,\phi,z,t)-\bar{v}_r(r,\phi,z,t)]dzd\phi drdt\Bigg\} \end{aligned}$$

$$\left\{1+\frac{\Theta V_0}{RL}+\frac{1}{\pi\Theta RL}\times\int_0^{\Theta}(\Theta-t)\int_0^{2\pi}\int_{-L}^{L}[v_r(R,\phi,z,\tau)-\bar{v}_r(R,\phi,z,\tau)]dzd\phi dt\right\}^{-1}\Bigg).$$

We determine the second-order approximations of temperature and concentrations of gases by using standard procedure of method of averaging of function corrections (see, for example, Sokolov 1955, Pankratov and Bulaeva 2016a, b) (1), Pankratov and Bulaeva (2016a, b) (2), Pankratov (2017a, b) (1), Pankratov (2017a, b) (2), Pankratov and Bulaeva (2013a) (1)), i.e., by replacing of required of these functions in right sides of Eqs. (12) and (13) on the following sums $T \to \alpha_{2T} + T_1$, $C \to \alpha_{i2C} + C_{i1}$. In this case the second-order approximations of the required functions could be written as

$$\begin{aligned}
&c\cdot T_2(r,\phi,z,t)\\
&=T_r+\lambda\int_0^t\frac{\partial^2 T_1(r,\phi,z,\tau)}{\partial r^2}d\tau+\lambda\frac{1}{r^2}\int_0^t\frac{\partial^2 T_1(r,\phi,z,\tau)}{\partial\phi^2}d\tau\\
&+\lambda\int_0^t\frac{\partial^2 T_1(r,\phi,z,\tau)}{\partial z^2}d\tau+\int_0^t p(r,\phi,z,\tau)d\tau\\
&-c\frac{\partial}{\partial r}\int_0^t\{[v_r(r,\phi,z,\tau)-\bar{v}_r(r,\phi,z,\tau)][\alpha_{2C}+C_{\Sigma 1}(r,\phi,z,\tau)][\alpha_{2T}+T_1(r,\phi,z,\tau)]\}d\tau\\
&-\frac{c}{r}\frac{\partial}{\partial\phi}\int_0^t\{[v_\phi(r,\phi,z,\tau)-\bar{v}_\phi(r,\phi,z,\tau)][\alpha_{2C}+C_{\Sigma 1}(r,\phi,z,\tau)][\alpha_{2T}+T_1(r,\phi,z,\tau)]\}d\tau\\
&-c\frac{\partial}{\partial z}\int_0^t\{[v_z(r,\phi,z,\tau)-\bar{v}_z(r,\phi,z,\tau)][\alpha_{2C}+C_{\Sigma 1}(r,\phi,z,\tau)][\alpha_{2T}+T_1(r,\phi,z,\tau)]\}d\tau
\end{aligned}\tag{17}$$

$$\begin{aligned}
&C_{21}(r,\phi,z,t)\\
&=\frac{1}{r}\frac{\partial}{\partial r}\int_0^t rD\frac{\partial C_{11}(r,\phi,z,\tau)}{\partial r}d\tau+\frac{1}{r^2}\frac{\partial}{\partial\phi}\int_0^t D\frac{\partial C_{11}(r,\phi,z,\tau)}{\partial\phi}d\tau\\
&+\frac{\partial}{\partial z}\int_0^t D\frac{\partial C_{11}(r,\phi,z,\tau)}{\partial z}d\tau-\alpha_{12C}\int_0^t k_1(r,\phi,z,\tau)[\alpha_{12C}+C_{11}(r,\phi,z,\tau)]d\tau\\
&-\frac{1}{r}\frac{\partial}{\partial r}\left\{r\int_0^t[\alpha_{12C}+C_{11}(r,\phi,z,\tau)]\cdot[v_r(r,\phi,z,\tau)-\bar{v}_r(r,\phi,z,\tau)]d\tau\right\}\\
&-\frac{1}{r}\frac{\partial}{\partial\phi}\int_0^t[\alpha_{12C}+C_{11}(r,\phi,z,\tau)]\cdot[v_\phi(r,\phi,z,\tau)-\bar{v}_\phi(r,\phi,z,\tau)]d\tau+C_0\delta(z+L)\\
&-\frac{\partial}{\partial z}\int_0^t[\alpha_{12C}+C_{11}(r,\phi,z,\tau)]\cdot[v_z(r,\phi,z,\tau)-\bar{v}_z(r,\phi,z,\tau)]d\tau
\end{aligned}\tag{18a}$$

$$\begin{aligned}
&C_{22}(r,\phi,z,t)\\
&=\frac{1}{r}\frac{\partial}{\partial r}\int_0^t rD\frac{\partial C_{11}(r,\phi,z,\tau)}{\partial r}d\tau+\frac{1}{r^2}\frac{\partial}{\partial\phi}\int_0^t D\frac{\partial C_{11}(r,\phi,z,\tau)}{\partial\phi}d\tau\\
&+\frac{\partial}{\partial z}\int_0^t D\frac{\partial C_{11}(r,\phi,z,\tau)}{\partial z}d\tau+C_0\delta(z+L)\\
&-\frac{1}{r}\frac{\partial}{\partial r}\left\{r\int_0^t[\alpha_{22C}+C_{21}(r,\phi,z,\tau)]\cdot[v_r(r,\phi,z,\tau)-\bar{v}_r(r,\phi,z,\tau)]d\tau\right\}
\end{aligned}\tag{18b}$$

$$
\begin{aligned}
&-\alpha_{22C}\int_0^t k_1(r,\phi,z,\tau)[\alpha_{22C}+C_{21}(r,\phi,z,\tau)]d\tau\\
&-\frac{1}{r}\frac{\partial}{\partial\phi}\int_0^t[\alpha_{22C}+C_{21}(r,\phi,z,\tau)]\cdot\left[v_\phi(r,\phi,z,\tau)-\bar{v}_\phi(r,\phi,z,\tau)\right]d\tau\\
&-\frac{\partial}{\partial z}\int_0^t[\alpha_{22C}+C_{21}(r,\phi,z,\tau)]\cdot[v_z(r,\phi,z,\tau)-\bar{v}_z(r,\phi,z,\tau)]d\tau
\end{aligned}
\tag{18b}
$$

$$
\begin{aligned}
&C_{32}(r,\phi,z,t)\\
&=\frac{1}{r}\frac{\partial}{\partial r}\int_0^t rD\frac{\partial C_{31}(r,\phi,z,\tau)}{\partial r}d\tau+\frac{1}{r^2}\frac{\partial}{\partial\phi}\int_0^t D\frac{\partial C_{31}(r,\phi,z,\tau)}{\partial\phi}d\tau\\
&+\frac{\partial}{\partial z}\int_0^t D\frac{\partial C_{31}(r,\phi,z,\tau)}{\partial z}d\tau+\alpha_{32C}\int_0^t k_3(r,\phi,z,\tau)[\alpha_{32C}+C_{31}(r,\phi,z,\tau)]d\tau\\
&-\frac{1}{r}\frac{\partial}{\partial r}\left\{r\int_0^t[\alpha_{32C}+C_{31}(r,\phi,z,\tau)]\cdot[v_r(r,\phi,z,\tau)-\bar{v}_r(r,\phi,z,\tau)]d\tau\right\}\\
&-\frac{1}{r}\frac{\partial}{\partial\phi}\int_0^t[\alpha_{32C}+C_{31}(r,\phi,z,\tau)]\cdot\left[v_\phi(r,\phi,z,\tau)-\bar{v}_\phi(r,\phi,z,\tau)\right]d\tau\\
&-\frac{\partial}{\partial z}\int_0^t[\alpha_{32C}+C_{31}(r,\phi,z,\tau)]\cdot[v_z(r,\phi,z,\tau)-\bar{v}_z(r,\phi,z,\tau)]d\tau.
\end{aligned}
\tag{18c}
$$

Average values of the second-order approximations of temperature and concentrations of gases α_{2T} and α_{2iC} were determined by standard relations

$$
\begin{aligned}
\alpha_{2T}&=\frac{1}{\pi\Theta R^2L}\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^L(T_2-T_1)dzd\phi drdt,\\
\alpha_{2C}&=\frac{1}{\pi\Theta R^2L}\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^L(C_2-C_1)dzd\phi drdt.
\end{aligned}
\tag{19}
$$

Substitution of the first- and the second-order approximations of temperature and concentrations in relations (18) gives a possibility to obtain relations for required average values

$$
\begin{aligned}
\alpha_{2T}=&\left(\frac{\lambda\sigma}{c\pi\Theta RL}\int_0^\Theta(\Theta-t)\int_0^{2\pi}\int_{-L}^L T^4(R,\phi,z,t)dzd\phi dt\right.\\
&-\frac{\lambda}{c\pi\Theta R^2L}\int_0^\Theta(\Theta-t)\int_0^{2\pi}\int_{-L}^L T_1(R,\phi,z,t)dzd\phi dt+\frac{\lambda}{c\pi\Theta R^2L}\\
&\times\int_0^\Theta(\Theta-t)\int_0^{2\pi}\int_{-L}^L T_1(0,\phi,z,t)dzd\phi dt\\
&-\frac{1}{\pi\Theta RL}\int_0^\Theta(\Theta-t)\int_0^{2\pi}\int_{-L}^L\{T_1(R,\phi,z,t)[\alpha_{2C}+C_{\Sigma1}(R,\phi,z,t)]-\alpha_{1T}\alpha_{1C}\}\\
&\times[v_r(R,\phi,z,t)-\bar{v}_r(R,\phi,z,t)]dzd\phi dt\\
&-\frac{1}{\pi\Theta R^2L}\int_0^\Theta(\Theta-t)\int_0^R\int_0^{2\pi}\int_{-L}^L T_1(r,\phi,z,t)\{[\alpha_{2C}+C_{\Sigma1}(r,\phi,z,t)]-\alpha_{1T}\alpha_{1C}\}\\
&\times[v_r(r,\phi,z,t)-\bar{v}_r(r,\phi,z,t)]dzd\phi rdrdt
\end{aligned}
$$

$$
\begin{aligned}
&-\frac{V_0}{\pi\Theta R^2 L}\int_0^{\Theta}(\Theta-t)\int_0^{R} r\int_0^{2\pi}[T_1(r,\phi,L,t)(\alpha_{2C}+C_0)-\alpha_{1T}\alpha_{1C}]d\phi drdt\\
&\times\left\{1+\frac{1}{\pi\Theta RL}\int_0^{\Theta}(\Theta-t)\int_0^{2\pi}\int_{-L}^{L}[v_r(R,\phi,z,t)-\bar{v}_r(R,\phi,z,t)]\sum_i[\alpha_{i2C}+C_{i1}(R,\phi,z,t)]\,dzd\phi dt\right.\\
&+2\Theta\left(\sum_i\alpha_{2iC}+C_0\right)\frac{V_0}{L}-\frac{1}{\pi\Theta R^2 L}\int_0^{\Theta}(\Theta-t)\int_0^{R} r\int_0^{2\pi}\int_{-L}^{L}[v_r(r,\phi,z,t)-\bar{v}_r(r,\phi,z,t)]\\
&\left.\int_0^{\Theta}(\Theta-t)\int_0^{R} r\int_0^{2\pi}\int_{-L}^{L}[v_r(r,\phi,z,t)-\bar{v}_r(r,\phi,z,t)]\cdot\sum_i[\alpha_{i2C}+C_{i1}(R,\phi,z,t)]\,dzd\phi drdt\right\}^{-1},
\end{aligned}
$$

$$
\alpha_{2iC}=\frac{1}{\pi\Theta R^2 L}\int_0^{\Theta}(\Theta-t)\int_0^{R} r\int_0^{2\pi}[C_{2i}(r,\phi,z,\tau)-C_{1i}(r,\phi,z,\tau)]d\phi drdt.
$$

3. Discussion

In this section, we will analyze the dynamics of mass and heat transfer during the growth of epitaxial layers from the gas phase in order to determine the conditions from which the properties of the epitaxial layers could be improved. In Fig. 2 shows the dependence of the concentration of the growth component on the frequency of rotation of the substrate. Curve 1 describes the dependence of the concentration of the growth component on the frequency of rotation of the substrate ω at atmospheric pressure without taking into account natural convection (at low growth temperatures, the value of natural convection can be neglected). Curve 2 describes the dependence of the concentration of the growth component on the frequency of rotation of the substrate at a reduced pressure by an order of magnitude without taking into account natural convection. Curve 3 describes the dependence of the concentration of the growth component on the frequency of rotation of the substrate at atmospheric pressure, taking into account natural convection. It follows from this figure that an increase in the rotational speed of the substrate leads to a more uniform distribution of the concentration of the material deposited on the substrate along its radius. An increase in the temperature of growth leads to an increase in the contribution of natural convection and a slowdown in the growth of epitaxial layers. In Fig. 3 shows the dependence of the concentration of the gas mixture on the diffusion coefficient *D*. Curve 1 describes the dependence of the concentration of the growth component on the diffusion coefficient at atmospheric pressure without taking into account natural convection. Curve 2 describes the dependence of the concentration of the growth component on the diffusion coefficient at atmospheric pressure with reduced pressure by an order of magnitude without taking into account natural convection. Curve 3 describes the dependence of the concentration of the growth component on the diffusion coefficient at atmospheric pressure at atmospheric pressure with allowance for natural convection. This figure shows a mono-ton decrease in the concentration under consideration. An increase in the value of the diffusion coefficient leads to an increase in the rate of transfer of the gas mixture, which leads to a decrease in its amount in the reaction zone. As a result, the growth rate of the epitaxial layer decreases. The value of the diffusion coefficient can be reduced by reducing the temperature of growth. However, with a decrease in growth temperature, the chemical reaction slows down. The dependence of the gas mixture concentration on the kinematic viscosity ν is shown in Fig. 4. The designations of the curves in this figure are the same as in the previous two. The decrease in concentration with an increase in viscosity is caused by a slower transfer of the gas mixture. The dependence of the concentration of

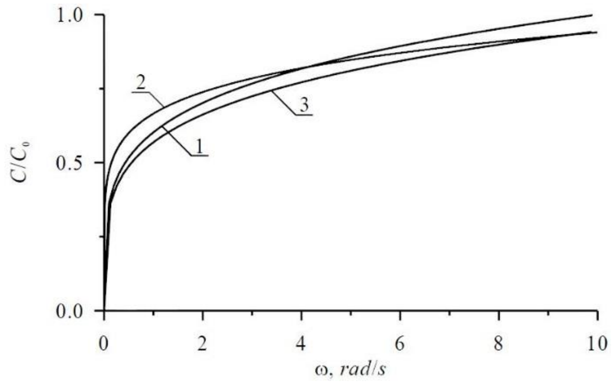


Fig. 2 The dependence of the concentration of the mixture of gases on the frequency of rotation of the substrate

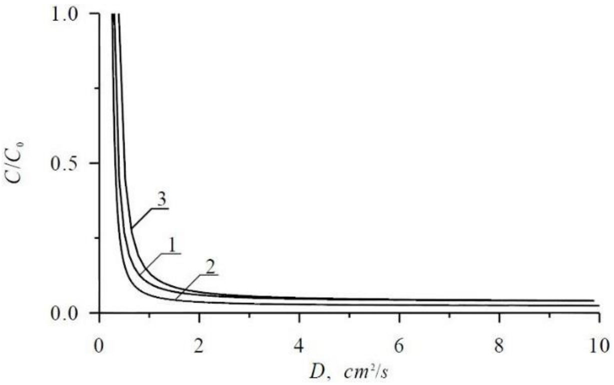


Fig. 3 The dependence of the concentration of the mixture of gases from its diffusion coefficient

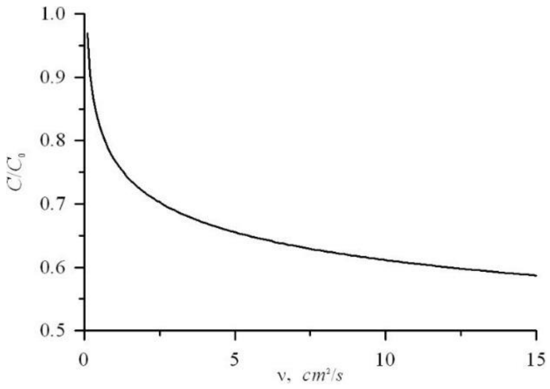


Fig. 4 The dependence of the concentration of the mixture of gases from the kinematic viscosity

the gas mixture on its velocity at the entrance to the reaction zone V_0 is shown in Fig. 5. Curve 1 describes the dependence of the concentration of the growth component on its velocity at the entrance to the reaction zone at atmospheric pressure without taking into account natural convection. Curve 2 describes the dependence of the concentration of the growth component on its velocity at

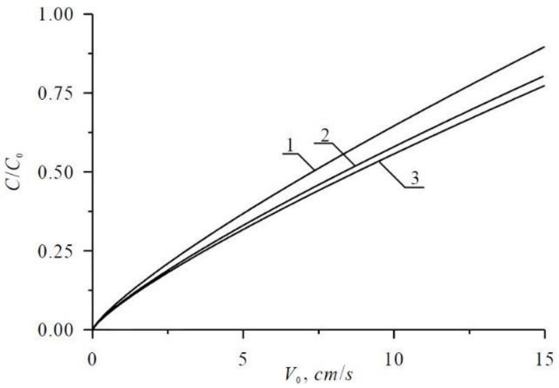


Fig. 5 The dependence of the concentration of the mixture of gases from its input velocity

the entrance to the reaction zone with pressure reduced by an order of magnitude without taking into account natural convection. Curve 3 describes the dependence of the concentration of the growth component on its velocity at the entrance to the reaction zone at atmospheric pressure, taking into account natural convection. An increase in the velocity of V_0 leads to an increase in the concentration of the gas mixture in the reaction zone and, as a consequence, to an acceleration of the growth of the epitaxial layer. From the analysis carried out it also follows that reducing the pressure in the reactor reduces the inertia of the processes occurring in it. Natural convection slows the growth of the epitaxial layer.

It should be noted that it is of interest to choose the power of induction heating of the zone of formation of the epitaxial layer in order to compensate for heat losses due to convective heat transfer (see, for example, Pankratov and Bulaeva 2015). In this case, the time for establishing the stationary mode of heating ϑ can be estimated in the framework of the previously proposed method (see, for example, Pankratov and Bulaeva 2013b) (2)) and has the value $\vartheta \approx (6\pi \quad -1)R^2/24\lambda_0$, where λ_0 is the average value of the thermal conductivity coefficient. In this case, the power required to compensate for the cooling of the region of the formation of the epitaxial layer can be estimated from the following relation $\int_0^R r \cdot p(r,\phi,z,t)dr \approx \sigma \cdot T^4(R,\phi,z,t) + \Theta \cdot v_z(R,\phi,z,t)/4\pi L R^2$ (Pankratov and Bulaeva 2016b).

4. Conclusions

In this paper, using the recently introduced analytical approach for the analysis of mass and heat transfer during film growth in reactors for epitaxy from the gas phase, these processes are analyzed taking into account natural convection and the possibility of changing the rate of chemical interaction between reagents. As a result of the analysis, the conditions under which the homogeneity of the grown epitaxial layers increases with a change in the values of the parameters of the growth process are formulated.

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