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A model for changing the technological process for the growth of epitaxial layers by means of the heating of the growth zone

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Abstract

The nonstationary transfer of heat during epitaxial layer growth in gas phase epitaxy reactors is analyzed within the work. Based on this analysis, several recommendations on the organization of the heating of the growth zone to increase the homogeneity of the epitaxial layers were formulated. An approach to analyze the transfer of heat during epitaxial layer growth from the gas phase is also introduced. The approach leads to the possibility of simultaneously accounting for heat transfer nonlinearity and changes of parameters of heat transfer in both space and time.

Keywords: epitaxy from gas phase, improvement of properties of films, analytical approach for modeling

1. Introduction

Currently, heterostructures are widely used to manufacture solid-state electronic devices. To grow the heterostructures, liquid and gas phase epitaxy, molecular beam epitaxy or magnetron sputtering are usually used. Many experimental results have been obtained to improve the manufacturing process of heterostructures e.g. Stepanenko (1980), Gusev and Gusev (1991), Lachin nad Savelov (2001), Vorob'ev et al. (2003), Sorokin et al. (2008), Lundin et al. (2009), Bravo-García et al. (2015), Li et al. (2006), Chakraborty et al. (2004), Taguchi et al. (2016), Mitsuhara (1998). At the same time, a smaller number of works address the prognosis of the considered technological processes Talalaev et al. (2001). Therefore, this paper presents the results of a numerical study focused on the evaluation of the variation of properties in growing epitaxial layers due to variations in the parameters of the technological process, taking into account native convection.

During the research, a gas phase epitaxy reactor for vertical growth was considered (see Fig. 1). The reactor consists of a substrate holder with a substrate, an external casing, a spiral around the casing in the area of the substrate to generate heating by induction for the activation of chemical reactions for the reagent's decay, and for epitaxial layer growth. A gaseous mixture of reagents and a gas-carrier enters the inlet of the reactor considered in Figure 1. The main goal of this paper is to analyze the variation of the properties of manufacturing epitaxial layers as a result of variation in the growth parameters considering native convection.

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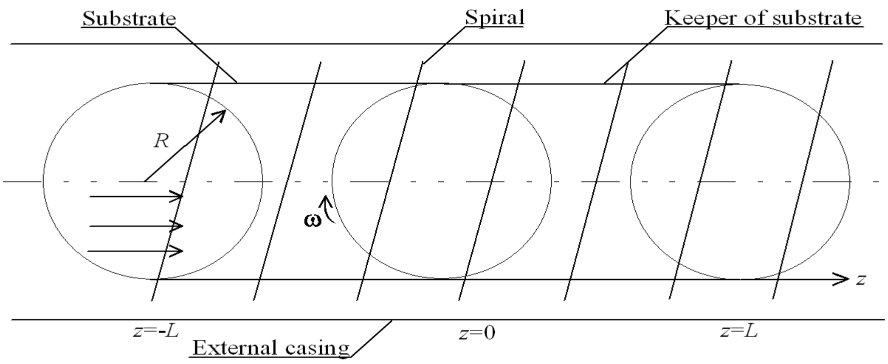

Fig. 1. A reactor for epitaxy from gas phase near zone of reaction

2. Method of solution

To obtain the required solution, the temperature distribution in space and time should be calculated. The considered distribution has been calculated as a solution of Fourier's second law in the following form by Carslaw and Jaeger (1964):

$$c\frac{\partial T(r,\phi,z,t)}{\partial t} = p(r,\phi,z,t) + div\left\{\lambda\cdot grad\left[T(r,\phi,z,t)\right] - \left[\vec{v}(r,\phi,z,t) - \bar{\vec{v}}(r,\phi,z,t)\right]\cdot c(T)\times T(r,\phi,z,t)\cdot C(r,\phi,z,t)\right\} \quad (1)$$

Here $\vec{v}$ describes the speed of flow of mixtures of gases; parameter c describes the capacity of heat; function $T(r, \phi, z, t)$ describes temperature distribution in space and time; function $p(r, \phi, z, t)$ describes power density in the considered system (substrate and keeper of the substrate); values r, ϕ and z are the coordinates of the cylindrical system; t is the current time; function $C(r, \phi, z, t)$ describes the distribution of concentration of the mixture of gases in space and time; value $\lambda = \bar{v}\bar{l}c_v\rho/3$ describes conductivity of heat; parameter $\bar{v} = \sqrt{2kT/m}$ describes the absolute value of the mean squared speed of molecules of gas; parameter $\bar{l}$ describes average value of free path of molecules of a considered mixture of gases between collisions; parameter c_v describes specific heat at a constant value of volume; parameter ρ describes the value of gas density.

The solution of the considered boundary value problem leads to the need to account for the movement of the gases-reagents and the gas-carrier with an account of the value of the concentration of the mixture. The required values are calculated by a solution of a system of equations: the Navier–Stokes equation and Fourier's second law. Also, the following approximation is assumed: the radius of substrate keeper R is essentially larger in comparison with the thickness of near-boundary and diffusion layers. We also consider a stream of gas as laminar. These assumptions lead to the need to solve the following system of equations:

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

$$\frac{\partial C(r,\phi,z,t)}{\partial t} = div\left\{D\cdot grad\left[C(r,\phi,z,t)\right] - \left[\vec{v}(r,\phi,z,t) - \bar{\vec{v}}\right]\cdot C(r,\phi,z,t)\right\} \quad (3)$$

Here parameter D describes the mixture of gases of diffusion coefficient; parameter P describes pressure in the considered reactor; parameter ρ describes the density of the considered gases; parameter ν describes kinematic viscosity. Now we consider the limiting flow regime. It is assumed that all molecules of deposited material, which are forthcoming to the substrate keeper, are being deposited on the considered substrate. We also consider homogenous and one dimension flow in this case. As a result, initial and boundary conditions can be written in the following form:

$C(r, \phi, -L, t) = C_0$, $C(r, \phi, 0, t) = 0$, $C(r, 0, z, t) = C(r, 2\pi, z, t)$, $C(r, \phi, z, 0) = C_0\delta(z + L)$, $C(0, \phi, z, t) \neq \infty$

$$\left.\frac{\partial C(r,\phi,z,t)}{\partial r}\right|_{r=R} = 0$$

$$\left.\frac{\partial C(r,\phi,z,t)}{\partial \phi}\right|_{\phi=0} = \left.\frac{\partial C(r,\phi,z,t)}{\partial \phi}\right|_{\phi=2\pi},\quad T(r,\phi,z,0) = T_r$$

$$v_r(r,\phi,0,t) = 0,\quad T(0,\phi,z,t) \neq \infty$$

$$-\lambda\left.\frac{\partial T(r,\phi,z,t)}{\partial r}\right|_{r=R} = \sigma T^4(R,\phi,z,t)$$

$$\left.\frac{\partial T(r,\phi,z,t)}{\partial \phi}\right|_{\phi=0} = \left.\frac{\partial T(r,\phi,z,t)}{\partial \phi}\right|_{\phi=2\pi}$$

$$T(r,0,z,t) = T(r,2\pi,z,t)$$

$$
\begin{gathered}
-\lambda \frac{\partial T(r,\phi,z,t)}{\partial z}\bigg|_{z=-L} = \sigma T^4(r,\phi,-L,t) \\
\frac{\partial v_r(r,\phi,z,t)}{\partial r}\bigg|_{r=0} = 0 \\
\frac{\partial v_\phi(r,\phi,z,t)}{\partial \phi}\bigg|_{\phi=0} = \frac{\partial v_\phi(r,\phi,z,t)}{\partial \phi}\bigg|_{\phi=2\pi} \\
\frac{\partial v_\phi(r,\phi,z,t)}{\partial \phi}\bigg|_{\phi=0} = \frac{\partial v_\phi(r,\phi,z,t)}{\partial \phi}\bigg|_{\phi=2\pi} \\
\frac{\partial v_r(r,\phi,z,t)}{\partial r}\bigg|_{r=R} = 0 \\
-\lambda \frac{\partial T(r,\phi,z,t)}{\partial z}\bigg|_{z=L} = \sigma T^4(r,\phi,z,t) \\
v_r(r,\phi,-L,t)=0, \\
v_r(r,\phi,L,t)=0,\ v_r(r,0,z,t)=v_r(r,2\pi,z,t), \\
v_r(0,\phi,z,t)\neq\infty,\ v_\phi(r,\phi,0,t)=\omega r, \\
v_\phi(r,\phi,-L,t)=0,\ v_\phi(r,\phi,L,t)=0, \\
v_\phi(r,0,z,t)=v_\phi(r,2\pi,z,t),\ v_\phi(0,\phi,z,t)\neq\infty, \\
v_z(r,\phi,-L,t)=V_0,\ v_z(r,\phi,0,t)=\overline{v}_z,\ v_z(r,\phi,L,t)=0, \\
v_z(r,0,z,t)=v_z(r,2\pi,z,t),\ v_z(0,\phi,z,t)\neq\infty, \\
v_r(r,\phi,z,0)=0,\ v_\phi(r,\phi,z,0)=0,\ v_z(r,\phi,-L,0)=V_0
\end{gathered} \tag{4}
$$

Here parameter σ is equal to $5.67 \cdot 10^{-8}$ W·m^{-2}·K^{-4}; parameter T_r is equal to room temperature; parameter ω describes the frequency of rotation of substrate.

Equations to calculate components of the velocity of flow in the cylindrical system of coordinate take the form:

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

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

$$
\begin{aligned}
\frac{\partial v_z}{\partial t} &= -v_r\frac{\partial v_r}{\partial r} - \frac{v_\phi}{r}\frac{\partial v_\phi}{\partial \phi} - v_z\frac{\partial v_z}{\partial z} + \\
&\nu\left(\frac{\partial^2 v_r}{\partial z^2} + \frac{\partial^2 v_z}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 v_z}{\partial \phi^2}\right) - \frac{\partial}{\partial z}\left(\frac{P}{\rho}\right)
\end{aligned} \tag{5c}
$$

The solution of the considered system of equations is calculated by the standard method of averaging of function corrections as in Sokolov (1955), Pankratov (2012), Pankratov and Bulaeva (2012; 2013a; 2013b; 2013c). Using the approach for the calculation of the first-order approximation of the considered components of the speed of mixture of gases flow, one should replace the required functions on their not yet known average values $v_r \to \alpha_{1r}$, $v_\phi \to \alpha_{1\phi}$, $v_z \to \alpha_{1z}$ on the right sides of the above equations of system (5). The replacement leads to the transformation of the above equations into the following form:

$$
\begin{aligned}
\frac{\partial v_{1r}}{\partial t} &= -\frac{\partial}{\partial r}\left(\frac{P}{\rho}\right) \\
\frac{\partial v_{1\phi}}{\partial t} &= -\frac{1}{r}\frac{\partial}{\partial \phi}\left(\frac{P}{\rho}\right) \\
\frac{\partial v_{1z}}{\partial t} &= -\frac{\partial}{\partial z}\left(\frac{P}{\rho}\right)
\end{aligned} \tag{6}
$$

Solutions of the above equations are the first-order approximations of the considered components:

$$
\begin{aligned}
v_{1r} &= -\frac{\partial}{\partial r}\int_0^t \frac{P}{\rho}\,d\tau \\
v_{1\phi} &= -\frac{1}{r}\frac{\partial}{\partial \phi}\int_0^t \frac{P}{\rho}\,d\tau \\
v_{1z} &= -\frac{\partial}{\partial z}\int_0^t \frac{P}{\rho}\,d\tau
\end{aligned} \tag{7}
$$

Approximations of second-order components of the speed of flow of a mixture of gases are obtained by the replacement of the considered functions by the sums $v_r \to \alpha_{1r}$, $v_\phi \to \alpha_{1\phi}$, $v_z \to \alpha_{1z}$. Approximations for the components could be written as:

$$
\begin{aligned}
\frac{\partial v_{2r}}{\partial t} &= \nu\left(\frac{\partial^2 v_{1r}}{\partial r^2} + \frac{\partial^2 v_{1r}}{\partial r\partial z} - \frac{\partial^2 v_{1r}}{\partial z^2} + \frac{\partial^2 v_{1z}}{\partial r\partial z}\right) - \\
&\frac{\partial}{\partial r}\left(\frac{P}{\rho}\right) - (\alpha_{2r} + v_{1r})\frac{\partial v_{1r}}{\partial r} - \frac{(\alpha_{2\phi} + v_{1\phi})}{r}\frac{\partial v_{1r}}{\partial \phi} - \\
&(\alpha_{2z} + v_{1z})\frac{\partial v_{1r}}{\partial z}
\end{aligned} \tag{8a}
$$

$$
\begin{aligned}
\frac{\partial v_{2\phi}}{\partial t} &= \nu\left(\frac{1}{r}\frac{\partial^2 v_{1r}}{\partial r\partial \phi} + \frac{2}{r^2}\frac{\partial^2 v_{1\phi}}{\partial \phi^2} - \frac{1}{r^2}\frac{\partial^2 v_{1r}}{\partial \phi\partial z} + \frac{\partial^2 v_{1\phi}}{\partial z^2}\right) - \\
&\frac{1}{r}\frac{\partial}{\partial \phi}\left(\frac{P}{\rho}\right) - (\alpha_{2r} + v_{1r})\frac{\partial v_{1\phi}}{\partial r} - \frac{(\alpha_{2\phi} + v_{1\phi})}{r}\frac{\partial v_{1\phi}}{\partial \phi} - \\
&(\alpha_{2z} + v_{1z})\frac{\partial v_{1\phi}}{\partial z}
\end{aligned} \tag{8b}
$$

$$
\begin{aligned}
\frac{\partial v_{2z}}{\partial t} &= \nu\left(\frac{\partial^2 v_{1r}}{\partial z^2} + \frac{\partial^2 v_{1z}}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 v_{1z}}{\partial \phi^2}\right) - \\
&\frac{\partial}{\partial z}\left(\frac{P}{\rho}\right) - (\alpha_{2r} + v_{1r})\frac{\partial v_{1z}}{\partial r} - \\
&\frac{(\alpha_{2\phi} + v_{1\phi})}{r}\frac{\partial v_{1z}}{\partial \phi} - (\alpha_{2z} + v_{1z})\frac{\partial v_{1z}}{\partial z}
\end{aligned} \tag{8c}
$$

To obtain the considered approximations, one should integrate the above equations with time. The integration leads to the following results:

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

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

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

Calculation of the averaged values α_{2r}, $\alpha_{2\phi}$, α_{2z} of the considered approximation can be done by the following standard relations:

$$\alpha_{2r}=\frac{1}{\pi\Theta R^2 L}\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^{L}\left(v_{2r}-v_{1r}\right)dz\,d\phi\,dr\,dt$$
$$\alpha_{2\phi}=\frac{1}{\pi\Theta R^2 L}\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^{L}\left(v_{2\phi}-v_{1\phi}\right)dz\,d\phi\,dr\,dt \tag{9}$$
$$\alpha_{2z}=\frac{1}{\pi\Theta R^2 L}\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^{L}\left(v_{2z}-v_{1z}\right)dz\,d\phi\,dr\,dt$$

Here parameter Θ describes continuance of technological process. Substitution of the considered approximations of the above components of speed to the above relation (9) leads to the possibility to obtain a system of three equations to calculate the above-average values:

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

Here:

$$A_1=1+\int_0^\Theta(\Theta-t)\int_0^R r\int_0^{2\pi}\int_{-L}^{L}\frac{\partial v_{1r}}{\partial r}dz\,d\phi\,dr\,dt$$

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

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

$$D_1=\nu\int_0^\Theta(\Theta-t)\times\int_0^R r\int_0^{2\pi}\int_{-L}^{L}\left(\frac{\partial^2 v_{1r}}{\partial r^2}+\frac{\partial^2 v_{1r}}{\partial r\partial z}-\frac{\partial^2 v_{1r}}{\partial z^2}+\frac{\partial^2 v_{1z}}{\partial r\partial z}\right)dz\,d\phi\,dr\,dt-\int_0^\Theta(\Theta-t)\int_0^R r\int_0^{2\pi}\int_{-L}^{L}v_{1r}\frac{\partial v_{1r}}{\partial r}dz\,d\phi\,dr\,dt-\frac{\pi}{8}\Theta^2\times R^2V_0^2-\int_0^\Theta(\Theta-t)\int_0^R\int_0^{2\pi}\int_{-L}^{L}v_{1\phi}\frac{\partial v_{1r}}{\partial \phi}dz\,d\phi\,dr\,dt$$

$$A_2=\int_0^\Theta(\Theta-t)\int_0^R r\int_0^{2\pi}\int_{-L}^{L}\frac{\partial v_{1r}}{\partial r}dz\,d\phi\,dr\,dt$$

$$B_2=\int_0^\Theta\int_0^R\int_0^{2\pi}\int_{-L}^{L}\frac{\partial v_{1r}}{\partial \phi}dz\,d\phi\,dr\cdot(\Theta-t)\,dt$$

$$D_2=\nu\int_0^\Theta(\Theta-t)\times\int_0^R r\int_0^{2\pi}\int_{-L}^{L}\left(\frac{1}{r}\frac{\partial^2 v_{1r}}{\partial r\partial \phi}+\frac{2}{r^2}\frac{\partial^2 v_{1\phi}}{\partial \phi^2}-\frac{1}{r^2}\frac{\partial^2 v_{1r}}{\partial\phi\partial z}+\frac{\partial^2 v_{1\phi}}{\partial z^2}\right)dz\,d\phi\,dr\,dt-\int_0^\Theta(\Theta-t)\int_0^R r\int_0^{2\pi}\int_{-L}^{L}v_{1r}\cdot\frac{\partial v_{1r}}{\partial r}dz\,d\phi\,dr\,dt-\frac{\pi}{8}\Theta^2R^2V_0^2-\int_0^\Theta(\Theta-t)\int_0^R\int_0^{2\pi}\int_{-L}^{L}v_{1\phi}\frac{\partial v_{1r}}{\partial \phi}dz\,d\phi\,dr\,dt$$

$$A_3=\int_0^\Theta(\Theta-t)\int_0^R r\int_0^{2\pi}\int_{-L}^{L}\frac{\partial v_{1z}}{\partial r}dz\,d\phi\,dr\,dt$$

$$B_3=\int_0^\Theta(\Theta-t)\int_0^R r\int_0^{2\pi}\int_{-L}^{L}\frac{\partial v_{1z}}{\partial \phi}dz\,d\phi\,dr\,dt$$

$$C_3=1+\frac{\pi}{2}\Theta^2R^2V_0$$

$$D_3=\nu\int_0^\Theta\int_0^R\int_0^{2\pi}\int_{-L}^{L}\left(\frac{\partial^2 v_{1r}}{\partial z^2}+\frac{\partial^2 v_{1z}}{\partial r^2}+\frac{1}{r^2}\frac{\partial^2 v_{1z}}{\partial \phi^2}\right)dz\,d\phi\times r\,dr(\Theta-t)\,dt-\int_0^\Theta(\Theta-t)\int_0^R r\int_0^{2\pi}\int_{-L}^{L}v_{1r}\frac{\partial v_{1z}}{\partial r}dz\,d\phi\,dr\,dt-\int_0^\Theta(\Theta-t)\int_0^R r\int_0^{2\pi}\int_{-L}^{L}v_{1\phi}\frac{\partial v_{1z}}{\partial \phi}dz\,d\phi\,dr\,dt-\frac{\pi}{8}\Theta^2R^2V_0^2$$

Solution of the considered system of equations (10) can be calculated by standard approaches for the solution of algebraic equations Korn and Korn (1968) and can be written in the following form:

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

Here:

$$\Delta = A_1\left(B_2C_3 - B_3C_2\right) - B_1\left(A_2C_3 - A_3C_2\right) + C_1\left(A_2B_3 - A_3B_2\right)$$

$$\Delta_r = D_1\left(B_2C_3 - B_3C_2\right) - B_1\left(D_2C_3 - D_3C_2\right) + C_1\left(D_2B_3 - D_3B_2\right)$$

$$\Delta_\phi = D_1\left(B_2C_3 - B_3C_2\right) - B_1\left(D_2C_3 - D_3C_2\right) + C_1\left(D_2B_3 - D_3B_2\right)$$

$$\Delta_z = A_1\left(B_2D_3 - B_3D_2\right) - B_1\left(A_2D_3 - A_3D_2\right) + D_1\left(A_2B_3 - A_3B_2\right)$$

In the present section, the components of the stream velocity of a mixture of gas-reagents and the gas-carrier which were used to grow the heterostructure are calculated using the second-order approximation of the standard method of averaging of function corrections. Usually, the considered approximation is sufficient to make a qualitative analysis of considered processes and obtain quantitative results. Now let us re-write equations (1) and (3) in a cylindrical system of coordinates:

$$c\frac{\partial T(r,\phi,z,t)}{\partial t} = \lambda\left[\frac{\partial^2 T(r,\phi,z,t)}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 T(r,\phi,z,t)}{\partial \phi^2} + \frac{\partial^2 T(r,\phi,z,t)}{\partial z^2}\right] - c\cdot\frac{\partial}{\partial r}\left\{C(r,\phi,z,t)\cdot T(r,\phi,z,t)\cdot\left[v_r(r,\phi,z,t) - \bar{v}_r(r,\phi,z,t)\right]\right\} - \frac{c}{r}\frac{\partial}{\partial \phi}\left\{\left[v_\phi(r,\phi,z,t) - \bar{v}_\phi(r,\phi,z,t)\right]\cdot C(r,\phi,z,t)\cdot T(r,\phi,z,t)\right\} - c\cdot\frac{\partial}{\partial z}\left\{\left[v_z(r,\phi,z,t) - \bar{v}_z(r,\phi,z,t)\right]\cdot C(r,\phi,z,t)\cdot T(r,\phi,z,t)\right\} + p(r,\phi,z,t) \quad (12)$$

$$\frac{\partial C(r,\phi,z,t)}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[rD\frac{\partial C(r,\phi,z,t)}{\partial r}\right] + \frac{1}{r^2}\frac{\partial}{\partial \phi}\left[D\frac{\partial C(r,\phi,z,t)}{\partial \phi}\right] + \frac{\partial}{\partial z}\left[D\frac{\partial C(r,\phi,z,t)}{\partial z}\right] - \frac{1}{r}\frac{\partial}{\partial r}\left\{rC(r,\phi,z,t)\cdot\left[v_r(r,\phi,z,t) - \bar{v}_r(r,\phi,z,t)\right]\right\} - \frac{1}{r}\frac{\partial}{\partial \phi}\left\{rC(r,\phi,z,t)\cdot\left[v_\phi(r,\phi,z,t) - \bar{v}_\phi(r,\phi,z,t)\right]\right\} - \frac{\partial}{\partial z}\left\{C(r,\phi,z,t)\cdot\left[v_z(r,\phi,z,t) - \bar{v}_z(r,\phi,z,t)\right]\right\} \quad (13)$$

To calculate the distribution of temperature field and concentration of a mixture of gases in space and time, we again have to use the method of the average of function corrections in the standard form. To calculate the first-order approximations of the above functions, one should replace their average values α_{1T} and α_{1C}, which are not yet known, on the right sides of the considered equations. Now let us use the aforementioned algorithm to obtain the first-order approximations of temperature and concentration of a mixture of gases:

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

$$C_1(r,\phi,z,t) = C_0 - \frac{\alpha_{1C}}{r}\int_0^t \frac{\partial\left\{r\left[v_r(r,\phi,z,\tau) - \bar{v}_r(r,\phi,z,\tau)\right]\right\}}{\partial r}d\tau - \frac{\alpha_{1C}}{r}\int_0^t \frac{\partial\left[v_\phi(r,\phi,z,\tau) - \bar{v}_\phi(r,\phi,z,\tau)\right]}{\partial \phi}d\tau + \frac{\alpha_{1C}}{r}\int_0^t \frac{\partial\left[v_\phi(r,\phi,z,\tau) - \bar{v}_\phi(r,\phi,z,\tau)\right]}{\partial \phi}d\tau - \alpha_{1C}\int_0^t \frac{\partial\left[v_z(r,\phi,z,\tau) - \bar{v}_z(r,\phi,z,\tau)\right]}{\partial z}d\tau \quad (15)$$

The recently considered but not yet known averaged value of temperature and components of the speed of gas flow can be calculated as:

$$\alpha_{1T} = \frac{1}{\pi\Theta R^2 L}\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^{L} T_1(r,\phi,z,\tau)\,dz\,d\phi\,dr\,dt$$

$$\alpha_{1C} = \frac{1}{\pi\Theta R^2 L}\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^{L} C_1(r,\phi,z,\tau)\,dz\,d\phi\,dr\,dt \quad (16)$$

Substitution of the above first-order approximations into the considered relations (16) leads to the following results of Korn and Korn (1968):

$$\alpha_{1C} = C_0 \Big/ L\cdot\left\{1 + \frac{1}{\pi\Theta RL}\int_0^\Theta(\Theta - t)\times\int_0^{2\pi}\int_{-L}^{L}\left[v_r(R,\phi,z,t) - \bar{v}_r(R,\phi,z,t)\right]dz\,d\phi\,dt + \frac{\Theta V_0}{RL}\right\}$$

$$\alpha_{1T} = \left[T_r + \frac{1}{\pi\Theta R^2 L}\int_0^\Theta (\Theta - t)\int_0^R r\int_0^{2\pi}\int_{-L}^{L}\frac{p(r,\phi,z,t)}{c}\,dz\,d\phi\,dr\,dt\right]\times$$
$$\left(1 + \frac{C_0}{\pi\Theta}\left\{\int_0^\Theta\int_0^{2\pi}\int_{-L}^{L}\left[v_r(R,\phi,z,\tau) - \bar{v}_r(R,\phi,z,\tau)\right]dz\,d\phi\,\times\right.\right.$$
$$\frac{(\Theta - t)}{RL^2}dt - \frac{1}{\pi\Theta R^2}\int_0^\Theta(\Theta - t)\times$$
$$\left.\int_0^R\int_0^{2\pi}\int_{-L}^{L}\left[v_r(r,\phi,z,t) - \bar{v}_r(r,\phi,z,t)\right]dz\,d\phi\,dr\,dt + \frac{V_0}{2}\right\}\times$$
$$\left\{1 + \frac{1}{\pi\Theta RL}\int_0^\Theta\int_0^{2\pi}\int_{-L}^{L}\left[\,v_r(R,\phi,z,\tau) - \right.\right.$$
$$\left.\left.\left.\bar{v}_r(R,\phi,z,\tau)\,\right]dz\,d\phi(\Theta - t)\,dt + \frac{\Theta V_0}{RL}\right\}^{-1}\right)$$

The second-order approximations of the considered functions are calculated with the standard method of averaging of function corrections as in Sokolov (1955), Pankratov (2012), Pankratov and Bulaeva (2012; 2013a; 2013b; 2013c). In this case, one should replace the considered functions on the right sides of the above equations (12) and (13) with the standard sums $T \to \alpha_{2T} + T_1$, $C \to \alpha_{2C} + C_1$. After the replacement, one obtains the second-order approximations of the considered functions in the following form:

$$c\cdot T_2(r,\phi,z,t) = \lambda\int_0^t \frac{\partial^2 T_1(r,\phi,z,\tau)}{\partial r^2}d\tau + \lambda\frac{1}{r^2}\int_0^t\frac{\partial^2 T_1(r,\phi,z,\tau)}{\partial\phi^2}d\tau +$$
$$\lambda\int_0^t\frac{\partial^2 T_1(r,\phi,z,\tau)}{\partial z^2}d\tau - c\cdot\frac{\partial}{\partial r}\int_0^t\left\{\left[\alpha_{2C} + C_1(r,\phi,z,\tau)\right]\times\right.$$
$$\left[v_r(r,\phi,z,\tau) - \bar{v}_r(r,\phi,z,\tau)\right]\cdot\left.\left[\alpha_{2T} + T_1(r,\phi,z,\tau)\right]\right\}d\tau - \tag{17}$$
$$\frac{c}{r}\frac{\partial}{\partial\phi}\int_0^t\left\{\left[\alpha_{2C} + C_1(r,\phi,z,\tau)\right]\cdot\left[v_\phi(r,\phi,z,\tau) - \bar{v}_\phi(r,\phi,z,\tau)\right]\times\right.$$
$$\left.\left[\alpha_{2T} + T_1(r,\phi,z,\tau)\right]\right\}d\tau - c\cdot\frac{\partial}{\partial z}\int_0^t\left\{\left[v_z(r,\phi,z,\tau) - \bar{v}_z(r,\phi,z,\tau)\right]\times\right.$$
$$\left.\left[\alpha_{2C} + C_1(r,\phi,z,\tau)\right]\cdot\left[\alpha_{2T} + T_1(r,\phi,z,\tau)\right]\right\}d\tau + T_r +$$
$$\int_0^t p(r,\phi,z,\tau)\,d\tau$$

$$-\frac{1}{r}\frac{\partial}{\partial r}\left\{r\int_0^t\left[\alpha_{2C} + C_1(r,\phi,z,\tau)\right]\times\right.$$
$$\left[v_r(r,\phi,z,\tau) - \bar{v}_r(r,\phi,z,\tau)\right]d\tau -$$
$$\frac{1}{r}\frac{\partial}{\partial\phi}\int_0^t\cdot\left[v_\phi(r,\phi,z,\tau) - \bar{v}_\phi(r,\phi,z,\tau)\right]\times \tag{18}$$
$$\left.\left[C_1(r,\phi,z,\tau) + +\alpha_{2C}\right]\right\}d\tau - \frac{\partial}{\partial z}\int_0^t\left[\alpha_{2C} + C_1(r,\phi,z,\tau)\right]\times$$
$$\left[v_z(r,\phi,z,\tau) - \bar{v}_z(r,\phi,z,\tau)\right]d\tau + C_0\delta(z + L)$$

Averaged values of the considered approximations of concentration and temperature of a mixture of gases α_{2C} and α_{2T} were calculated with these standard relations (19):

$$\alpha_{2T} = \frac{1}{\pi\Theta R^2 L}\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^{L}(T_2 - T_1)\,dz\,d\phi\,dr\,dt$$
$$\alpha_{2C} = \frac{1}{\pi\Theta R^2 L}\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^{L}(C_2 - C_1)\,dz\,d\phi\,dr\,dt \tag{19}$$

Substitution of both approximations of the concentration of a mixture of gases and temperature into equations (19) helps to obtain equations for the calculation of the required averaged values of the considered functions:

$$\alpha_{2T} = \left(\frac{\lambda\sigma}{c\pi\Theta RL}\int_0^\Theta(\Theta - t)\int_0^{2\pi}\int_{-L}^{L}T^4(R,\phi,z,t)\,dz\,d\phi\,dt - \right.$$
$$\frac{\lambda\sigma}{c\pi\Theta R^2 L}\int_0^\Theta(\Theta - t)\int_0^{2\pi}\int_{-L}^{L}T_1(R,\phi,z,t)\,dz\,d\phi\,dt + \frac{\lambda\sigma}{c\pi\Theta R^2 L}\times$$
$$\int_0^\Theta(\Theta - t)\int_0^{2\pi}\int_{-L}^{L}T_1(0,\phi,z,t)\,dz\,d\phi\,dt -$$
$$\frac{1}{\pi\Theta RL}\int_0^\Theta(\Theta - t)\int_0^{2\pi}\int_{-L}^{L}\left\{\left[\alpha_{2C} + C_1(R,\phi,z,t)\right] - \alpha_{1T}\alpha_{1C}\right\}\times$$
$$\left[v_r(R,\phi,z,t) - \bar{v}_r(R,\phi,z,t)\right]\cdot T_1(R,\phi,z,t)\,dz\,d\phi\,dt -$$
$$\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^{L}\left\{T_1(r,\phi,z,t)\left[\alpha_{2C} + C_1(r,\phi,z,t)\right] - \alpha_{1T}\alpha_{1C}\right\}\times$$
$$\left[v_r(r,\phi,z,t) - \bar{v}_r(r,\phi,z,t)\right]dz\,d\phi\,dr\,\times$$
$$\frac{(\Theta - t)\,dt}{\pi\Theta R^2 L} - \frac{V_0}{\pi\Theta R^2 L}\int_0^\Theta(\Theta - t)\int_0^R r\,\times$$
$$\int_0^{2\pi}\left[T_1(r,\phi,L,t)(\alpha_{2C} + C_0) - \alpha_{1T}\alpha_{1C}\right]d\phi\,dr\,dt\,\times$$
$$\left\{\frac{1}{\pi\Theta RL}\int_0^\Theta\int_0^{2\pi}\int_{-L}^{L}\left[\alpha_{2C} + C_1(R,\phi,z,t)\right]\times\right.$$
$$\left[v_r(R,\phi,z,t) - \bar{v}_r(R,\phi,z,t)\right]dz\,d\phi(\Theta - t)\,dt +$$
$$1 - \frac{1}{\pi\Theta R^2 L}\int_0^\Theta(\Theta - t)\int_0^R r\int_0^{2\pi}\int_{-L}^{L}\left[v_r(r,\phi,z,t) - \bar{v}_r(r,\phi,z,t)\right]\times$$
$$\left.\left[\,\alpha_{2C} + C_1(r,\phi,z,t)\,\right]dz\,d\phi\,dr\,dt + 2\Theta V_0\left(\alpha_{2C} + C_0\right)L^{-1}\right\}^{-1}$$

$$\alpha_{2C} = \frac{1}{\pi\Theta R^2 L}\int_0^\Theta(\Theta - t)\int_0^R r\,\times$$
$$\int_0^{2\pi}D\left[\left.\frac{\partial C_1(r,\phi,z,\tau)}{\partial z}\right|_{z=L} - \left.\frac{\partial C_1(r,\phi,z,\tau)}{\partial z}\right|_{z=-L}\right]d\phi\,dr\,dt -$$
$$\frac{1}{\pi\Theta R^2 L}\int_0^\Theta(\Theta - t)\int_0^{2\pi}\int_{-L}^{L}\left\{r\left[\alpha_{2C} - \alpha_{1C} + C_1(R,\phi,z,\tau)\right]\times\right.$$
$$\left.\left[v_r(R,\phi,z,\tau) - \bar{v}_r(R,\phi,z,\tau)\right]\right\}dz\,d\phi\,dt -$$
$$\frac{V_0}{\pi\Theta R^2 L}\int_0^\Theta(\Theta - t)\int_0^R r\int_0^{2\pi}\left(\alpha_{2C} - \alpha_{1C} + C_0\right)dz\,d\phi\,dr\,dt$$

3. Discussion

In this section, heat and mass transfer during epitaxial layer growth is analyzed to formulate conditions to increase the homogeneity of layers. Figure 2 presents the dependences of temperature on time in the reactor under low- and high-frequency (curves 1 and 2, respectively) and induction heating conditions, respectively. From this figure it is clear that the growth temperature reaches its stationary value more rapidly with high-frequency heating. In this case, a shorter growth time of the epitaxial layer is achieved, as well as a more stable composition can be provided. In this case it is necessary to change the growth temperature before the finishing of the process due to the greater stability of the rate of interaction between the reactants. Figure 3 shows the dependences of the heating temperature in the reaction zone on the value of the axial coordinate at various values of the velocity of the considered mixture of gases at the inlet to the reactor. These figures show that increasing the considered velocity leads to a decrease in temperature (a probable reason for this would be convective heat transfer) in the growth zone of the epitaxial layer and its area, bringing it closer to the value that existed in the reactor before the start of the technological process. In the considered situation it is possible to properly select the power of the induction heating of the zone of growth of the epitaxial layer in order to compensate for heating losses due to convective heating transfer, as noted by Pankratov and Bulaeva (2015). In this case, the time for achievement of the stationary heating regime ϑ can be estimated by the previously introduced approach by Pankratov and Bulaeva (2013c) and has the value $\vartheta \approx (6\pi - 1)R^2/24\lambda_0$, where λ_0 is the average value of the thermal conductivity. In this case, the power required to compensate the cooling of the region of growth of the epitaxial layer can be estimated from the relation

$$\int_0^R r \cdot p(r,\phi,z,t)\, dr \approx$$

$$\sigma \cdot T^4(R,\phi,z,t) + \Theta \cdot v_z(R,\phi,z,t) / 4\pi LR^2$$

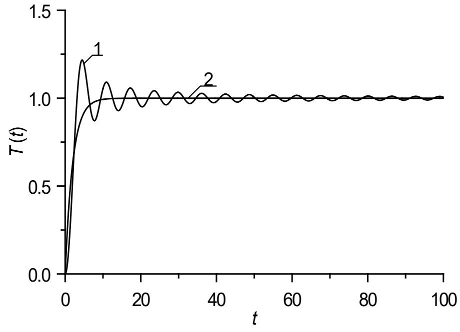

Fig. 2. Dependences of temperature on time for different types of heating: low-frequency (curve 1) and high-frequency (curve 2)

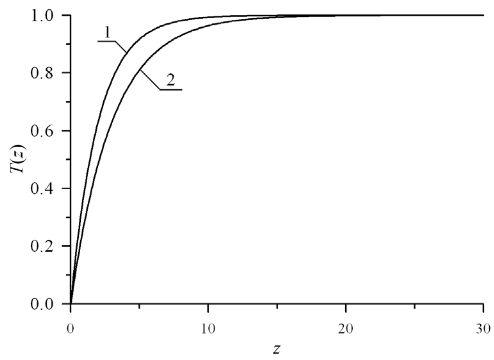

Fig. 3. Dependences of temperature on coordinates for different values of the speed of the gas mixture at the inlet of the reactor: at a lower speed (curve 1) and at a higher speed (curve 2)

Conclusion

In this paper, the nonstationary growth of films during epitaxy from the gas phase was analyzed. The analysis provides the possibility to formulate some recommendations for the organization of the heating of the growth zone in order to increase the homogeneity of the epitaxial layers. An analytical approach for the analysis of heat and mass transfer during the considered growth of films from the gas phase was also introduced. The approach has the ability to simultaneously take into account the nonlinearity of mass and heat transfer, as well as changes in their parameters in space and time at a given moment.

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