Variation of properties of films during growth in a vertical reactor for gas phase epitaxy with variation of parameters of technological process with account native convection

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ABSTRACT

In this paper we analyzed mass and heat transport during growth films in a vertical reactors for gas phase epitaxy with account native convection by using recently introduced analytical approach for prognosis of the above processes. Native convection takes a significant influence on growth of films at high temperature. We determine several conditions to increase homogeneity of epitaxial layers with varying parameters of technological process.   © 2016 Trade Science Inc. - INDIA

KEYWORDS

Gas phase epitaxy;
Native convection;
Increasing of homogeneity of films;
Analytical approach for modeling.

INTRODUCTION

In the present time different heterostructures are using to manufacture solid state electronic devices. The most common methods for growing heterostructures are epitaxy from gas and liquid phase, magnetron sputtering, molecular beam epitaxy. Their are many experimental works describe manufacturing and growth of heterostructures[1-11]. At the same time essentially smaller quantity of works describes prognosis of epitaxy processes[12]. Main aim of the present paper is prognosis changing of properties of growing of epitaxial layers with changing of parameters of technological process with account native convection.

In this paper we consider a vertical reactor for gas phase epitaxy (see Figure 1). The reactor con-

sist of an external casing, keeper of substrate with a substrate and a spiral around the casing in area of the substrate to generate induction heating to activate chemical reactions of decay of reagents and to growth of the epitaxial layer. A mixture of gas reagents and gas-carrier inputs into inlet of the reactor from Figure 1. Main aim of the present paper is analysis of changing of properties of growing epitaxial layers with changing parameters of growth with account native convection.

Method of solution

To solve our aims we determine spatio-temporal distribution of temperature. We determine the spatio-temporal distribution as solution of the following the second Fourier law[13]

$$c\frac{\partial T(r,\varphi,z,t)}{\partial t} = p(r,\varphi,z,t) + div\{\lambda \cdot grad[T(r,\varphi,z,t)] -$$

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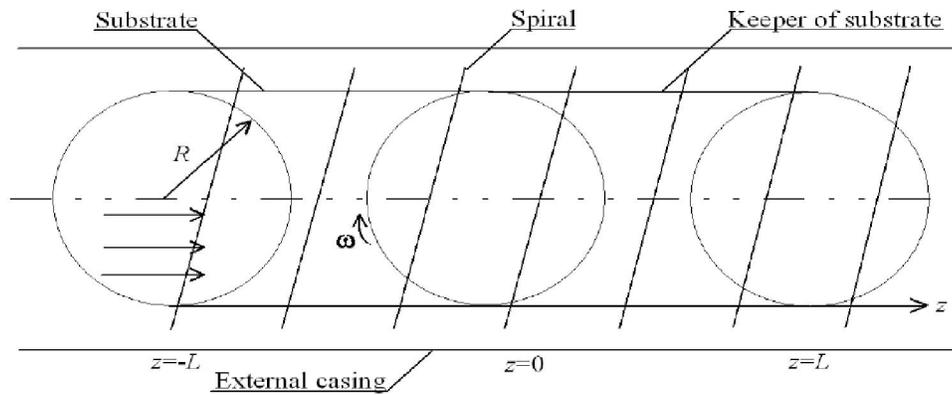**Figure 1 : A reactor for the gas phase epitaxy in neighborhoods of reaction zone**

$$-\left[\vec{v}\left(r,\varphi,z,t\right)-\vec{\vec{v}}\left(r,\varphi,z,t\right)\right]\cdot c\left(T\right)\cdot T\left(r,\varphi,z,t\right)\cdot C\left(r,\varphi,z,t\right)\},$$ (1)

where $\vec{v}$ is the speed of flow of mixture of gases; c is the heat capacity; T (r,φ,z,t) is the spatio-temporal distribution of temperature; p (r,φ,z,t) is the density of power in the system substrate - keeper of substrate; r, , z and t are the cylindrical coordinates and time; C (r,φ,z,t) is the spatio-temporal distribution of concentration of mixture of gases; λ is the heat conductivity. Value of heat conductivity could be determine

by the following relation: $\lambda = \dfrac{1}{3}\bar{v}\bar{l}c_{v}\rho$, where $\bar{v}$ is the modulus of mean squared speed of the gas

molecules, which equal to $\bar{v} = \sqrt{2kT/m}$, $\bar{l}$ is the average free path of gas molecules between colli-

sions, c_{v} is the specific heat at constant volume, ρ is the density of gas.

To solve this boundary problem we shall take into account moving of mixture of gases and concentration of the mixture. We determine the required values by solving the equation of Navier-Stokes and the second Fourier law. We also assume that radius of keeper of substrate R essentially larger, than thickness of diffusion and near-boundary layers. We also assume, that stream of gas is laminar. In this situation the appropriate equations could be written as

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

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

where D is the diffusion coefficient of mixture of gases (gases-reagents and gas- carrier); P is the pressure; ρ is the density; ν is the kinematic viscosity. Let us consider the regime of the limiting flow, when all forthcoming to the disk molecules of deposit material are deposing on the substrate, flow is homogenous and one dimension. In this case boundary and initial conditions could be written as

C (r,φ,-L,t) = C$_0$, C (r,φ,0,t) = 0, C (r,0,z,t) = C (r,2π,z,t), C (r,φ,z,0) = C$_0$δ (z+L),

$$C\left(0,\varphi,z,t\right) \neq \infty, \quad \left.\frac{\partial C\left(r,\varphi,z,t\right)}{\partial r}\right|_{r=R} = 0, \quad \left.\frac{\partial C\left(r,\varphi,z,t\right)}{\partial \varphi}\right|_{\varphi=0} = \left.\frac{\partial C\left(r,\varphi,z,t\right)}{\partial \varphi}\right|_{\varphi=2\pi}, \quad T\,(r,\varphi,z,0) = T_{r},$$

$$-\lambda\left.\frac{\partial T\left(r,\varphi,z,t\right)}{\partial r}\right|_{r=R} = \sigma T^{4}\left(R,\varphi,z,t\right), \quad \left.\frac{\partial T\left(r,\varphi,z,t\right)}{\partial \varphi}\right|_{\varphi=0} = \left.\frac{\partial T\left(r,\varphi,z,t\right)}{\partial \varphi}\right|_{\varphi=2\pi},$$

$$-\lambda \frac{\partial T(r,\varphi,z,t)}{\partial z}\bigg|_{z=-L} = \sigma T^4(r,\varphi,-L,t), \quad T(r,0,z,t) = T(r,2\pi,z,t), \quad \frac{\partial v_r(r,\varphi,z,t)}{\partial r}\bigg|_{r=0} = 0,$$

$$\frac{\partial v_\varphi(r,\varphi,z,t)}{\partial \varphi}\bigg|_{\varphi=0} = \frac{\partial v_\varphi(r,\varphi,z,t)}{\partial \varphi}\bigg|_{\varphi=2\pi}, \quad \frac{\partial v_\varphi(r,\varphi,z,t)}{\partial \varphi}\bigg|_{\varphi=0} = \frac{\partial v_\varphi(r,\varphi,z,t)}{\partial \varphi}\bigg|_{\varphi=2\pi}, \quad (4)$$

$$\frac{\partial v_r(r,\varphi,z,t)}{\partial r}\bigg|_{r=R} = 0, \quad -\lambda \frac{\partial T(r,\varphi,z,t)}{\partial z}\bigg|_{z=L} = \sigma T^4(r,\varphi,z,t), \quad T(0,\varphi,z,t) \neq \infty, \quad v_r(r,\varphi,-L,t) = 0,$$

$v_r(r,\varphi,0,t) = 0$, $v_r(r,\varphi,L,t) = 0$, $v_r(r,0,z,t) = v_r(r,2\pi,z,t)$, $v_r(0,\varphi,z,t) \neq \infty$, $v_\varphi(r,\varphi,0,t) = \omega r$,
$v_\varphi(r,\varphi,-L,t) = 0$, $v_\varphi(r,\varphi,L,t) = 0$, $v_\varphi(r,0,z,t) = v_\varphi(r,2\pi,z,t)$, $v_\varphi(0,\varphi,z,t) \neq \infty$, $v_z(r,\varphi,-L,t) = V_0$,
$v_z(r,\varphi,0,t) = \overline{v}_z$, $v_z(r,\varphi,L,t) = 0$, $v_z(r,0,z,t) = v_z(r,2\pi,z,t)$, $v_z(0,\varphi,z,t) \neq$, $v_r(r,\varphi,z,0) = 0$,
$v_\varphi(r,\varphi,z,0) = 0$, $v_z(r,\varphi,-L,0) = V_0$,
where $\sigma = 5,67 \cdot 10^{-8}$ W·m^{-2}·K^{-4}, T_r is the room temperature, ω is the frequency of rotation of substrate. Value of velocity of mixture of gases in the end of reactor (for $z = L$) has been chosen as zero to decrease energy cost during growth of heterostructure.

Equations for components of velocity of flow with account cylindrical system of coordinate could be written as

$$\frac{\partial v_r}{\partial t} = -v_r \frac{\partial v_r}{\partial r} - \frac{v_\varphi}{r}\frac{\partial v_\varphi}{\partial \varphi} - v_z \frac{\partial v_z}{\partial z} + \nu\left(\frac{\partial^2 v_r}{\partial r^2} + \frac{\partial^2 v_r}{\partial r \partial z} - \frac{\partial^2 v_r}{\partial z^2} + \frac{\partial^2 v_z}{\partial r \partial z}\right) - \frac{\partial}{\partial r}\left(\frac{P}{\rho}\right) \quad \textbf{(5a)}$$

$$\frac{\partial v_\varphi}{\partial t} = -v_r \frac{\partial v_r}{\partial r} - \frac{v_\varphi}{r}\frac{\partial v_\varphi}{\partial \varphi} - v_z \frac{\partial v_z}{\partial z} +$$

$$+\nu\left(\frac{1}{r}\frac{\partial^2 v_r}{\partial r \partial \varphi} + \frac{2}{r^2}\frac{\partial^2 v_\varphi}{\partial \varphi^2} - \frac{1}{r^2}\frac{\partial^2 v_r}{\partial \varphi \partial z} + \frac{\partial^2 v_\varphi}{\partial z^2}\right) - \frac{1}{r}\frac{\partial}{\partial \varphi}\left(\frac{P}{\rho}\right) \quad \textbf{(5b)}$$

$$\frac{\partial v_z}{\partial t} = -v_r \frac{\partial v_r}{\partial r} - \frac{v_\varphi}{r}\frac{\partial v_\varphi}{\partial \varphi} - v_z \frac{\partial v_z}{\partial z} + \nu\left(\frac{\partial^2 v_r}{\partial z^2} + \frac{\partial^2 v_z}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 v_z}{\partial \varphi^2}\right) - \frac{\partial}{\partial z}\left(\frac{P}{\rho}\right). \quad \textbf{(5c)}$$

We determine solution of this system of equations by using of method of averaging of function corrections[14-19]. Framework this approach to determine the first-order approximation of components of speed of flow of mixture of gases we replace of the required functions on their average values $v_r \to \alpha_{1r}$, $v_\varphi \to \alpha_{1\varphi}$, $v_z \to \alpha_{1z}$ in right sides of equations of system (5). After the replacement we obtain equations for the first-order approximations of the components

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

Solutions of the above equations could be written as

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

The second-order approximations of components of speed of flow could be obtain by replacement of the required functions on the following sums $v_r \to \alpha_{1r}$, $v_\varphi \to \alpha_{1\varphi}$, $v_z \to \alpha_{1z}$. Approximations for the components could be written as

$$\frac{\partial v_{2r}}{\partial t} = \nu \left(\frac{\partial^2 v_{1r}}{\partial r^2} + \frac{\partial^2 v_{1r}}{\partial r \partial z} - \frac{\partial^2 v_{1r}}{\partial z^2} + \frac{\partial^2 v_{1z}}{\partial r \partial z} \right) - \frac{\partial}{\partial r}\left(\frac{P}{\rho} \right) -$$

$$- \left(\alpha_{2r} + v_{1r} \right)\frac{\partial v_{1r}}{\partial r} - \frac{\left(\alpha_{2\varphi} + v_{1\varphi} \right)}{r}\frac{\partial v_{1r}}{\partial \varphi} - \left(\alpha_{2z} + v_{1z} \right)\frac{\partial v_{1r}}{\partial z}, \tag{8a}$$

$$\frac{\partial v_{2\varphi}}{\partial t} = \nu \left(\frac{1}{r}\frac{\partial^2 v_{1r}}{\partial r \partial \varphi} + \frac{2}{r^2}\frac{\partial^2 v_{1\varphi}}{\partial \varphi^2} - \frac{1}{r^2}\frac{\partial^2 v_{1r}}{\partial \varphi \partial z} + \frac{\partial^2 v_{1\varphi}}{\partial z^2} \right) - \frac{1}{r}\frac{\partial}{\partial \varphi}\left(\frac{P}{\rho} \right) -$$

$$- \left(\alpha_{2r} + v_{1r} \right)\frac{\partial v_{1\varphi}}{\partial r} - \frac{\left(\alpha_{2\varphi} + v_{1\varphi} \right)}{r}\frac{\partial v_{1\varphi}}{\partial \varphi} - \left(\alpha_{2z} + v_{1z} \right)\frac{\partial v_{1\varphi}}{\partial z}, \tag{8b}$$

$$\frac{\partial v_{2z}}{\partial t} = \nu \left(\frac{\partial^2 v_{1r}}{\partial z^2} + \frac{\partial^2 v_{1z}}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 v_{1z}}{\partial \varphi^2} \right) - \frac{\partial}{\partial z}\left(\frac{P}{\rho} \right) -$$

$$- \left(\alpha_{2r} + v_{1r} \right)\frac{\partial v_{1z}}{\partial r} - \frac{\left(\alpha_{2\varphi} + v_{1\varphi} \right)}{r}\frac{\partial v_{1z}}{\partial \varphi} - \left(\alpha_{2z} + v_{1z} \right)\frac{\partial v_{1z}}{\partial z}. \tag{8c}$$

Integration of the above equations leads to the following result

$$v_{2r} = \nu \int\limits_0^t \left(\frac{\partial^2 v_{1r}}{\partial r^2} + \frac{\partial^2 v_{1r}}{\partial r \partial z} - \frac{\partial^2 v_{1r}}{\partial z^2} + \frac{\partial^2 v_{1z}}{\partial r \partial z} \right) d\tau - \frac{\partial}{\partial r}\left(\int\limits_0^t \frac{P}{\rho} d\tau \right) -$$

$$- \int\limits_0^t \left(\alpha_{2r} + v_{1r} \right)\frac{\partial v_{1r}}{\partial r} d\tau - \int\limits_0^t \frac{\left(\alpha_{2\varphi} + v_{1\varphi} \right)}{r}\frac{\partial v_{1r}}{\partial \varphi} d\tau - \int\limits_0^t \left(\alpha_{2z} + v_{1z} \right)\frac{\partial v_{1r}}{\partial z} d\tau, \tag{8d}$$

$$v_{2\varphi} = \nu \int\limits_0^t \left(\frac{1}{r}\frac{\partial^2 v_{1r}}{\partial r \partial \varphi} + \frac{2}{r^2}\frac{\partial^2 v_{1\varphi}}{\partial \varphi^2} - \frac{1}{r^2}\frac{\partial^2 v_{1r}}{\partial \varphi \partial z} + \frac{\partial^2 v_{1\varphi}}{\partial z^2} \right) d\tau - \frac{1}{r}\frac{\partial}{\partial \varphi}\left(\int\limits_0^t \frac{P}{\rho} d\tau \right) -$$

$$- \int\limits_0^t \left(\alpha_{2r} + v_{1r} \right)\frac{\partial v_{1\varphi}}{\partial r} d\tau - \int\limits_0^t \frac{\left(\alpha_{2\varphi} + v_{1\varphi} \right)}{r}\frac{\partial v_{1\varphi}}{\partial \varphi} d\tau - \int\limits_0^t \left(\alpha_{2z} + v_{1z} \right)\frac{\partial v_{1\varphi}}{\partial z} d\tau, \tag{8e}$$

$$v_{2z} = \nu \int\limits_0^t \left(\frac{\partial^2 v_{1r}}{\partial z^2} + \frac{\partial^2 v_{1z}}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 v_{1z}}{\partial \varphi^2} \right) d\tau - \frac{\partial}{\partial z}\left(\int\limits_0^t \frac{P}{\rho} d\tau \right) -$$

$$- \int\limits_0^t \left(\alpha_{2r} + v_{1r} \right)\frac{\partial v_{1z}}{\partial r} d\tau - \int\limits_0^t \frac{\left(\alpha_{2\varphi} + v_{1\varphi} \right)}{r}\left(\alpha_{2\varphi} + v_{1\varphi} \right)\frac{\partial v_{1z}}{\partial \varphi} d\tau - \int\limits_0^t \left(\alpha_{2z} + v_{1z} \right)\frac{\partial v_{1z}}{\partial z} d\tau. \tag{8f}$$

We determine average values α_{2r}, $\alpha_{2\varphi}$, α_{2z} by the following relations

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$$\alpha_{2r} = \frac{1}{\pi \Theta R^2 L} \int\limits_0^\Theta \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^L (v_{2r} - v_{1r}) \, dz \, d\varphi \, dr \, dt,$$

$$\alpha_{2\varphi} = \frac{1}{\pi \Theta R^2 L} \int\limits_0^\Theta \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^L (v_{2\varphi} - v_{1\varphi}) \, dz \, d\varphi \, dr \, dt, \tag{9}$$

$$\alpha_{2z} = \frac{1}{\pi \Theta R^2 L} \int\limits_0^\Theta \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^L (v_{2z} - v_{1z}) \, dz \, d\varphi \, dr \, dt,$$

where Θ is the continuance of moving of mixture of gases through reactor. Substitution of the first- and the second-order approximations of the required components of speed into the relation (9) give us possibility to obtain system of equations to determine required average values

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

where $A_1 = 1 + \int\limits_0^\Theta (\Theta - t) \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^L \frac{\partial v_{1r}}{\partial r} \, dz \, d\varphi \, dr \, dt$, $B_1 = \int\limits_0^\Theta (\Theta - t) \int\limits_0^R \int\limits_0^{2\pi} \int\limits_{-L}^L \frac{\partial v_{1r}}{\partial \varphi} \, dz \, d\varphi \, dr \, dt$,

$C_1 = C_2 = \frac{\pi}{2} \Theta^2 R^2 V_0$, $D_1 = v \int\limits_0^\Theta \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^L \left(\frac{\partial^2 v_{1r}}{\partial r^2} + \frac{\partial^2 v_{1r}}{\partial r \partial z} - \frac{\partial^2 v_{1r}}{\partial z^2} + \frac{\partial^2 v_{1z}}{\partial r \partial z} \right) dz \, d\varphi \, dr \, (\Theta -$

$- t) \, dt - \frac{\pi}{8} \Theta^2 R^2 V_0^2 - \int\limits_0^\Theta (\Theta - t) \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^L v_{1r} \frac{\partial v_{1r}}{\partial r} \, dz \, d\varphi \, dr \, dt - \int\limits_0^\Theta \int\limits_0^R \int\limits_0^{2\pi} \int\limits_{-L}^L v_{1\varphi} \frac{\partial v_{1r}}{\partial \varphi} \, dz \, d\varphi \, dr \times$

$\times (\Theta - t) dt$, $A_2 = \int\limits_0^\Theta (\Theta - t) \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^L \frac{\partial v_{1r}}{\partial r} \, dz \, d\varphi \, dr \, dt$, $B_2 = 1 + \int\limits_0^\Theta \int\limits_0^R \int\limits_0^{2\pi} \int\limits_{-L}^L \frac{\partial v_{1r}}{\partial \varphi} \, dz \, d\varphi \, dr \, (\Theta -$

$- t) dt$, $D_2 = v \int\limits_0^\Theta (\Theta - t) \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^L \left(\frac{1}{r} \frac{\partial^2 v_{1r}}{\partial r \partial \varphi} + \frac{2}{r^2} \frac{\partial^2 v_{1\varphi}}{\partial \varphi^2} - \frac{1}{r^2} \frac{\partial^2 v_{1r}}{\partial \varphi \partial z} + \frac{\partial^2 v_{1\varphi}}{\partial z^2} \right) dz \, d\varphi \, dr \, dt -$

$- \int\limits_0^\Theta (\Theta - t) \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^L v_{1r} \frac{\partial v_{1r}}{\partial r} \, dz \, d\varphi \, dr \, dt - \frac{\pi}{8} \Theta^2 R^2 V_0^2 - \int\limits_0^\Theta (\Theta - t) \int\limits_0^R \int\limits_0^{2\pi} \int\limits_{-L}^L v_{1\varphi} \frac{\partial v_{1r}}{\partial \varphi} \, dz \, d\varphi \, dr \, dt$,

$A_3 = \int\limits_0^\Theta (\Theta - t) \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^L \frac{\partial v_{1z}}{\partial r} \, dz \, d\varphi \, dr \, dt$, $B_3 = \int\limits_0^\Theta (\Theta - t) \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^L \frac{\partial v_{1z}}{\partial \varphi} \, dz \, d\varphi \, dr \, dt$, $C_3 = 1 +$

$+ \frac{\pi}{2} \Theta^2 R^2 V_0$, $D_3 = v \int\limits_0^\Theta (\Theta - t) \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^L \left(\frac{\partial^2 v_{1r}}{\partial z^2} + \frac{\partial^2 v_{1z}}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2 v_{1z}}{\partial \varphi^2} \right) dz \, d\varphi \, dr \, dt - \int\limits_0^\Theta (\Theta - t) \times$

$$\times \int_0^R r \int_0^{2\pi} \int_{-L}^L v_{1r} \frac{\partial v_{1z}}{\partial r} d z d \varphi d r d t - \int_0^\Theta (\Theta - t) \int_0^R r \int_0^{2\pi} \int_{-L}^L v_{1\varphi} \frac{\partial v_{1z}}{\partial \varphi} d z d \varphi d r d t - \frac{\pi}{8} \Theta^2 R^2 V_0^2 .$$

Solution of the above system of equations could be determined by standard approaches[19] and could be written as

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

where $\Delta = A_1(B_2 C_3 - B_3 C_2) - B_1(A_2 C_3 - A_3 C_2) + C_1(A_2 B_3 - A_3 B_2)$, $\Delta_r = D_1(B_2 C_3 - B_3 C_2) -$

$- B_1(D_2 C_3 - D_3 C_2) + C_1(D_2 B_3 - D_3 B_2)$, $\Delta_\varphi = D_1(B_2 C_3 - B_3 C_2) - B_1(D_2 C_3 - D_3 C_2) + C_1 \times$

$\times (D_2 B_3 - D_3 B_2)$, $\Delta_z = A_1(B_2 D_3 - B_3 D_2) - B_1(A_2 D_3 - A_3 D_2) + D_1(A_2 B_3 - A_3 B_2)$.

In this section we obtained components of velocity of stream of mixture of materials in gas phase, which are used for growth of heterostructure, and gas-carrier in the second-order approximation framework method of averaging of function corrections. Usually the second-order approximation is enough good approximation to make qualitative analysis of obtained solution and to obtain some quantitative results.

Let us re-write Eqs.(1) and (3) by using cylindrical system of coordinate

$$c \frac{\partial T(r,\varphi,z,t)}{\partial t} = \lambda \left[\frac{\partial^2 T(r,\varphi,z,t)}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2 T(r,\varphi,z,t)}{\partial \varphi^2} + \frac{\partial^2 T(r,\varphi,z,t)}{\partial z^2} \right] - c \cdot \frac{\partial}{\partial r} \{C(r,\varphi,z,t) \cdot$$

$$\cdot T(r,\varphi,z,t) \cdot [v_r(r,\varphi,z,t) - \bar{v}_r(r,\varphi,z,t)]\} - \frac{c}{r} \frac{\partial}{\partial \varphi} \{[v_\varphi(r,\varphi,z,t) - \bar{v}_\varphi(r,\varphi,z,t)] \cdot C(r,\varphi,z,t) \cdot$$

$$\cdot T(r,\varphi,z,t)\} - c \cdot \frac{\partial}{\partial z} \{[v_z(r,\varphi,z,t) - \bar{v}_z(r,\varphi,z,t)] \cdot C(r,\varphi,z,t) \cdot T(r,\varphi,z,t)\} + p(r,\varphi,z,t), \tag{12}$$

$$\frac{\partial C(r,\varphi,z,t)}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left[r D \frac{\partial C(r,\varphi,z,t)}{\partial r} \right] + \frac{1}{r^2} \frac{\partial}{\partial \varphi} \left[D \frac{\partial C(r,\varphi,z,t)}{\partial \varphi} \right] +$$

$$+ \frac{\partial}{\partial z} \left[D \frac{\partial C(r,\varphi,z,t)}{\partial z} \right] - \frac{1}{r} \frac{\partial}{\partial r} \{r C(r,\varphi,z,t) \cdot [v_r(r,\varphi,z,t) - \bar{v}_r(r,\varphi,z,t)]\} -$$

$$- \frac{1}{r} \frac{\partial}{\partial \varphi} \{r C(r,\varphi,z,t) \cdot [v_\varphi(r,\varphi,z,t) - \bar{v}_\varphi(r,\varphi,z,t)]\} -$$

$$- \frac{\partial}{\partial z} \{C(r,\varphi,z,t) \cdot [v_z(r,\varphi,z,t) - \bar{v}_z(r,\varphi,z,t)]\}. \tag{13}$$

To determine spatio-temporal distribution of temperature and concentration of gas mixture we used method of average of function corrections. To determine the first- order approximations of the required functions we replace them on their not yet known average values α_{1T} and α_{1C} in right sides of the above equations. Farther we used recently consider algorithm to obtain the first-order approximations of temperature and concentration of gas mixture

$$T_1(r,\varphi,z,t) = T_r + \int_0^t \frac{p(r,\varphi,z,\tau)}{c} d\tau - \alpha_{1T} \alpha_{1C} \int_0^t \frac{\partial [v_r(r,\varphi,z,\tau) - \bar{v}_r(r,\varphi,z,\tau)]}{\partial r} d\tau -$$

$$- \frac{\alpha_{1T} \alpha_{1C}}{r} \int_0^t \frac{\partial [v_\varphi(r,\varphi,z,\tau) - \bar{v}_\varphi(r,\varphi,z,\tau)]}{\partial \varphi} d\tau - \alpha_{1T} \alpha_{1C} \int_0^t \frac{\partial [v_z(r,\varphi,z,\tau) - \bar{v}_z(r,\varphi,z,\tau)]}{\partial z} d\tau, \tag{14}$$

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$$C_1(r,\varphi,z,t) = C_0 - \frac{\alpha_{1C}}{r}\int_0^t \frac{\partial\{r[v_r(r,\varphi,z,\tau)-\bar{v}_r(r,\varphi,z,\tau)]\}}{\partial r}d\tau -$$

$$-\frac{\alpha_{1C}}{r}\int_0^t \frac{\partial[v_\varphi(r,\varphi,z,\tau)-\bar{v}_\varphi(r,\varphi,z,\tau)]}{\partial\varphi}d\tau - \alpha_{1C}\int_0^t \frac{\partial[v_z(r,\varphi,z,\tau)-\bar{v}_z(r,\varphi,z,\tau)]}{\partial z}d\tau. \qquad (15)$$

The above not yet known average values could be determined by the standard relations

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

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

Substitution of the first-order approximations of temperature and concentration of gas mixter into relations (16) gives us the following results[20]

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

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

$$\times\int_0^{2\pi}\int_{-L}^L[v_r(R,\varphi,z,\tau)-\bar{v}_r(R,\varphi,z,\tau)]\,dz\,d\varphi\,dt-\int_0^\Theta\int_0^R\int_0^{2\pi}\int_{-L}^L[v_r(r,\varphi,z,t)-\bar{v}_r(r,\varphi,z,t)]dz\,d\varphi\,dr\times$$

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

$$+1+\Theta V_0/RL\bigg\}^{-1}\bigg).$$

The second-order approximations of temperature and concentration of mixture of gases we determine framework the method of averaging of function corrections[14-19], i.e. by replacement of the required functions in right sides of equations (12) and (13) on the following sums $T\to\alpha_{2T}+T_1$, $C\to\alpha_{2C}+C_1$. In this case the second-order approximations of the above required functions could be written as

$$c\cdot T_2(r,\varphi,z,t) = \lambda\int_0^t \frac{\partial^2 T_1(r,\varphi,z,\tau)}{\partial r^2}d\tau + \lambda\frac{1}{r^2}\int_0^t \frac{\partial^2 T_1(r,\varphi,z,\tau)}{\partial\varphi^2}d\tau + \lambda\int_0^t \frac{\partial^2 T_1(r,\varphi,z,\tau)}{\partial z^2}d\tau +$$

$$-c\cdot\frac{\partial}{\partial r}\int_0^t \{[v_r(r,\varphi,z,\tau)-\bar{v}_r(r,\varphi,z,\tau)]\cdot[\alpha_{2C}+C_1(r,\varphi,z,\tau)]\cdot[\alpha_{2T}+T_1(r,\varphi,z,\tau)]\}d\tau -$$

$$-\frac{c}{r}\frac{\partial}{\partial\varphi}\int_0^t \{[\alpha_{2C}+C_1(r,\varphi,z,\tau)]\cdot[v_\varphi(r,\varphi,z,\tau)-\bar{v}_\varphi(r,\varphi,z,\tau)]\cdot[\alpha_{2T}+T_1(r,\varphi,z,\tau)]\}d\tau -$$

$$-c\cdot\frac{\partial}{\partial z}\int_0^t \{[v_z(r,\varphi,z,\tau)-\bar{v}_z(r,\varphi,z,\tau)]\cdot[\alpha_{2C}+C_1(r,\varphi,z,\tau)]\cdot[\alpha_{2T}+T_1(r,\varphi,z,\tau)]\}d\tau +$$

$$+\int_0^t p(r,\varphi,z,\tau)d\tau+T_r, \qquad (17)$$

$$C_2(r,\varphi,z,t) = \frac{1}{r}\frac{\partial}{\partial r}\int_0^t rD\frac{\partial C_1(r,\varphi,z,\tau)}{\partial r}d\tau + \frac{1}{r^2}\frac{\partial}{\partial \varphi}\int_0^t D\frac{\partial C_1(r,\varphi,z,\tau)}{\partial \varphi}d\tau +$$

$$+\frac{\partial}{\partial z}\int_0^t D\frac{\partial C_1(r,\varphi,z,\tau)}{\partial z}d\tau - \frac{1}{r}\frac{\partial}{\partial r}\left\{r\int_0^t[\alpha_{2C}+C_1(r,\varphi,z,\tau)]\cdot[v_r(r,\varphi,z,\tau)-\bar{v}_r(r,\varphi,z,\tau)]d\tau\right\} -$$

$$-\frac{1}{r}\frac{\partial}{\partial \varphi}\int_0^t[\alpha_{2C}+C_1(r,\varphi,z,\tau)]\cdot[v_\varphi(r,\varphi,z,\tau)-\bar{v}_\varphi(r,\varphi,z,\tau)]d\tau + C_0\delta(z+L) -$$

$$-\frac{\partial}{\partial z}\int_0^t[\alpha_{2C}+C_1(r,\varphi,z,\tau)]\cdot[v_z(r,\varphi,z,\tau)-\bar{v}_z(r,\varphi,z,\tau)]d\tau \,. \tag{18}$$

Averages values of the second-order approximations of temperature and concentration of mixture α_{2T} and α_{2C} have been calculated by using the following standard relations

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

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

Substitution of the first- and the second-order approximations of temperature and concentration of mixture into relations (18) gives us possibility to obtain equations to determine required average values

$$\alpha_{2T} = \left(\frac{\lambda\sigma}{c\pi\Theta RL}\int_0^\Theta(\Theta-t)\int_0^{2\pi}\int_{-L}^L T^4(R,\varphi,z,t)\,dz\,d\varphi\,dt - \int_0^\Theta(\Theta-t)\int_0^{2\pi}\int_{-L}^L T_1(R,\varphi,z,t)\,dz\,d\varphi\,dt \times\right.$$

$$\times\frac{\lambda}{c\pi\Theta R^2L}+\frac{\lambda}{c\pi\Theta R^2L}\int_0^\Theta(\Theta-t)\int_0^{2\pi}\int_{-L}^L T_1(0,\varphi,z,t)\,dz\,d\varphi\,dt - \int_0^\Theta(\Theta-t)\int_0^{2\pi}\int_{-L}^L\{T_1(R,\varphi,z,t)\times$$

$$\times[\alpha_{2C}+C_1(R,\varphi,z,t)]-\alpha_{1T}\alpha_{1C}\}[v_r(R,\varphi,z,t)-\bar{v}_r(R,\varphi,z,t)]\,dz\,d\varphi\,dt\frac{1}{\pi\Theta RL}-\frac{1}{\pi\Theta R^2L}\times$$

$$\times\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^L\{T_1(r,\varphi,z,t)[\alpha_{2C}+C_1(r,\varphi,z,t)]-\alpha_{1T}\alpha_{1C}\}\cdot[v_r(r,\varphi,z,t)-\bar{v}_r(r,\varphi,z,t)]\,dz\,d\varphi\,dr\times$$

$$\times(\Theta-t)\,dt-\frac{V_0}{\pi\Theta R^2L}\int_0^\Theta(\Theta-t)\int_0^R r\int_0^{2\pi}[T_1(r,\varphi,L,t)(\alpha_{2C}+C_0)-\alpha_{1T}\alpha_{1C}]\,d\varphi\,dr\,dt\left\{\frac{1}{\pi\Theta RL}\times\right.$$

$$\times\int_0^\Theta(\Theta-t)\int_0^{2\pi}\int_{-L}^L[v_r(R,\varphi,z,t)-\bar{v}_r(R,\varphi,z,t)][\alpha_{2C}+C_1(R,\varphi,z,t)]\,dz\,d\varphi\,dt+1-\frac{1}{\pi\Theta R^2L}\times$$

$$\times\int_0^\Theta(\Theta-t)\int_0^R r\int_0^{2\pi}\int_{-L}^L[v_r(r,\varphi,z,t)-\bar{v}_r(r,\varphi,z,t)]\cdot[\alpha_{2C}+C_1(r,\varphi,z,t)]\,dz\,d\varphi\,dr\,dt+(\alpha_{2C}+C_0)\times$$

$$+2\Theta V_0/L\}^{-1} \,,$$

$$\alpha_{2C} = \frac{1}{\pi\Theta R^2L}\int_0^\Theta(\Theta-t)\int_0^R r\int_0^{2\pi}D\left[\left.\frac{\partial C_1(r,\varphi,z,\tau)}{\partial z}\right|_{z=L}-\left.\frac{\partial C_1(r,\varphi,z,\tau)}{\partial z}\right|_{z=-L}\right]\,d\varphi\,dr\,dt-$$

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$$-\int_0^\Theta (\Theta - t) \int_0^{2\pi} \int_{-L}^{L} \left\{ r \left[\alpha_{2C} - \alpha_{1C} + C_1(R, \varphi, z, \tau) \right] \cdot \left[v_r(R, \varphi, z, \tau) - \bar{v}_r(R, \varphi, z, \tau) \right] \right\} dz \, d\varphi \, dt \times$$

$$\times \frac{1}{\pi \Theta R^2 L} - \frac{V_0}{\pi \Theta R^2 L} \int_0^\Theta (\Theta - t) \int_0^R r \int_0^{2\pi} \left(\alpha_{2C} - \alpha_{1C} + C_0 \right) dz \, d\varphi \, dr \, dt .$$

DISCUSSION

In the present paper we analyzed dynamics of mass and heat transport during growth of epitaxial layers from gas phase to determine conditions to improvement of properties of epitaxial layers. Figure 2 shows dependence of concentration of material of epitaxial layer on frequency of rotation of substrate. Curve 1 describes dependence of concentration of reagents on the frequency of rotation of substrate at atmospheric pressure without taking into account native convection (at low temperature of growth one can neglect by native convection). Curve 2 describes dependence of concentration of reagents on the frequency of rotation
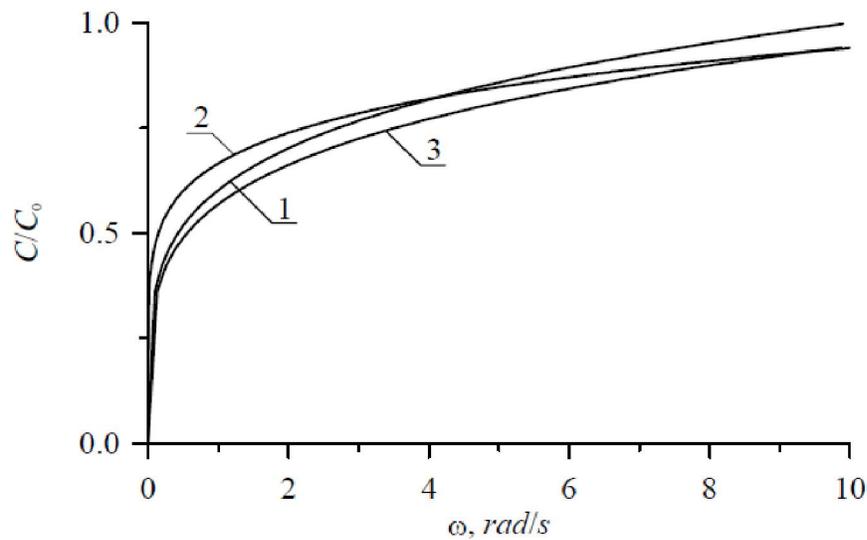

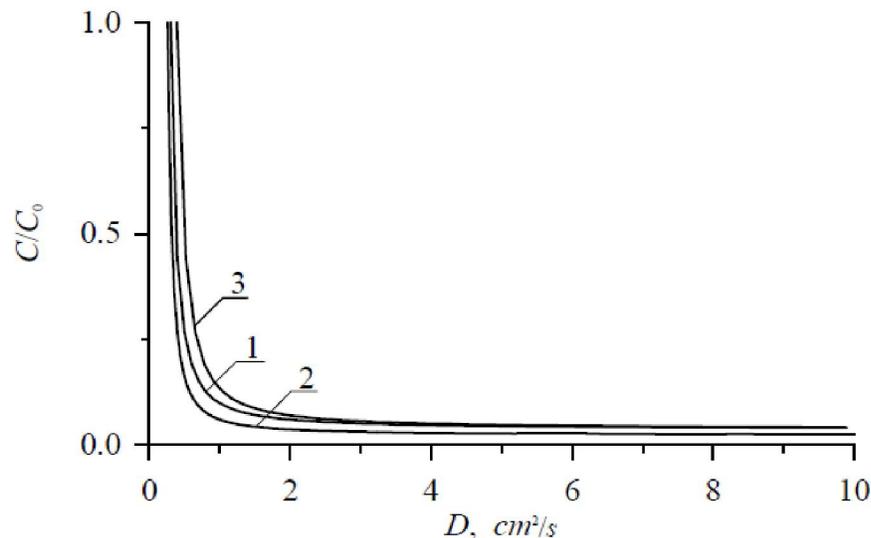**Figure 2 : Dependence of concentration of mixture of gases on frequency of rotation of substrate**

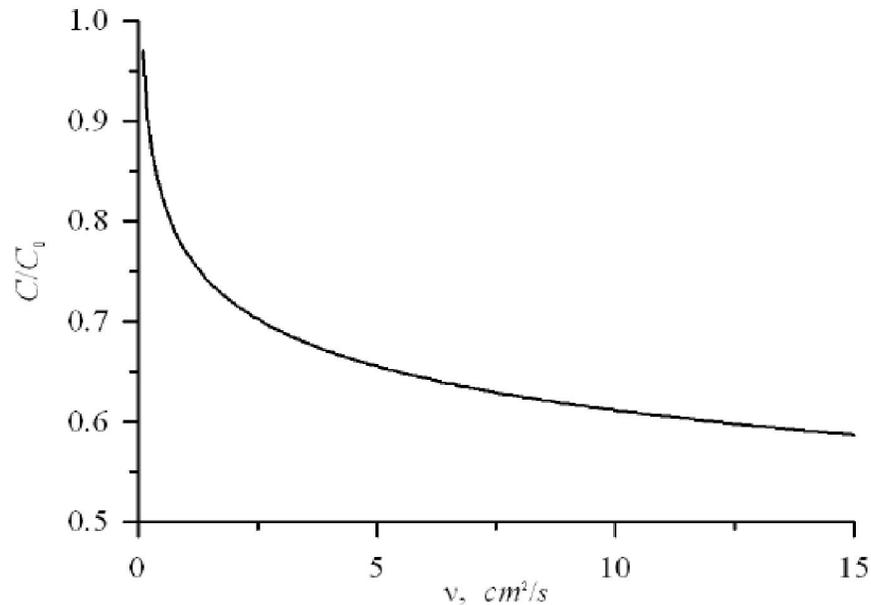**Figure 3 : Dependence of concentration of mixture of gases on diffusion coefficient**

Figure 4 : Dependence of concentration of mixture of gases on kinematical viscosity ν
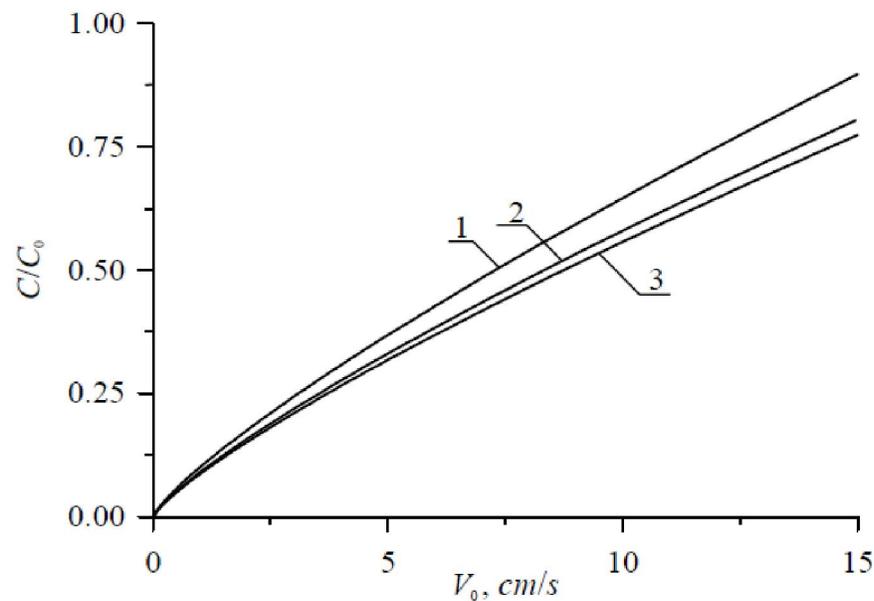

Figure 5 : Dependence of concentration of mixture of gases on inlet speed

of substrate at low pressure (10 % of atmospheric pressure) without taking into account native convection. Curve 3 describes dependence of concentration of reagents on the frequency of rotation of substrate at atmospheric pressure with account native convection. Increasing of temperature of growth leads to increasing of influence of native convection on growth process. The Figure 2 shows, that increasing of frequency of rotation of substrate leads to more homogenous distribution of concentration deposited on the substrate material on radius of the substrate. The Figure 3 shows, that concentration of concentration of material of epitaxial layer on diffusion coefficient D. Curve 1 describes dependence of concentration of reagents on the diffusion coefficient at atmospheric pressure without taking into account native convection. Curve 2 describes dependence of concentration of reagents on the diffusion coefficient at low pressure (10 % of atmospheric pressure) without taking into account native convection. Curve 3 describes dependence of concentration of reagents on the diffusion coefficient at atmo-

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spheric pressure with account native convection. The figure shows monotonous decreasing of the considered concentration. Increasing of value of diffusion coefficient leads to increasing of speed of transport of gases leads to decreasing of quantity of reagents in reaction zone due to high speed of gases. In this case one can obtain decreasing of speed of growth of epitaxial layer. Value of diffusion coefficient could be decreased by decreasing of temperature of grown. However decreasing of temperature of grown leads to deceleration of chemical reaction.

Dependence of concentration of mixture of gases on kinematical viscosity ν is presented on Figure 4. Designations curves in this figure are the same as in the previous two. Decreasing of the concentration with increasing of the viscosity is a reason of deceleration of gas transport. Dependence of the considered concentration on inlet speed of gases V_0 is presented on Figure 5. Curve 1 describes dependence of concentration of reagents on the speed V_0 at atmospheric pressure without taking into account native convection. Curve 2 describes dependence of concentration of reagents on the speed V_0 at low pressure (10 % of atmospheric pressure) without taking into account native convection. Curve 3 describes dependence of concentration of reagents on the speed V_0 at atmospheric pressure with account native convection. Increasing of the speed V_0 leads to increasing of concentration of reagents in reaction zone and to increasing of speed of growth of epitaxial layers.

The above analysis shows, that decreasing of pressure in the reactor leads to reducing the inertness of the considered processes of mass and heat transport. Native convection leads to deceleration of growth of epitaxial layers. It should be also noted, that it is attracted an interest choosing of value of power of induction heating of growth area to compensate heat loss due to convective heat[21]. In this case heating time ϑ could be estimated framework recently introduced approach[22] and could be calculated as $\vartheta \approx (6\pi - 1)R^2/24\lambda_0$, where λ_0 is the average value of heat conductivity. In this case power, which is necessary for compensation losing of heat during manufacturing of epitaxial layer, could be estimated by using the following relation:

$$\int_0^R r \cdot p(r,\varphi,z,t)\, d\, r \approx \sigma \cdot T^4(R,\varphi,z,t) + \Theta \cdot v_z(R,\varphi,z,t)/4\pi\, LR^2.$$

CONCLUSION

In the present paper we analyzed dependences of dynamics of mass and heat transport in reactors for epitaxy from gas phase on physical and technological parameters. We compare growth regimes at atmospheric and at low pressure and analyzed influence of native convection on growth of epitaxial layers. Accounting the calculated results it have been formulated recommendations to improve properties of epitaxial layers.

ACKNOWLEDGMENTS

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