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Analysis of regimes of growth of epitaxial layers in gas phase epitaxy reactors to increase homogeneity of properties of the layers

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ABSTRACT

In this paper we analyzed mass and heat transport during growth of epitaxial layers in reactors for epitaxy from gas phase with sloping keeper of substrate in comparison with flow of mixture of gas-carrier and gas-reagents. We analyzed possibility to increase homogeneity of properties of epitaxial layers during different regimes of growth. We introduce an analytical approach for analysis of technological process.

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INTRODUCTION

Wide using multilayer structures for manufacturing of solid state electronic devices leads to necessity to improve properties of layers of the structures. In the present time following procedures are using for growth multilayer structures: molecular-beam epitaxy, epitaxy from gas phase, magnetron sputtering. One could find a lot quantity of experimental works about growth of heterostructures^[1-10]. However essentially smaller quantity works describe any prognosis of epitaxy^[10].

In this paper to generalize recently published results^[11-16] we analyzed processes of mass and heat reactors for epitaxy from gas phase with sloping keeper of substrate under angle ψ with direction of flow of gas-reagents. Main aim of our paper is determination conditions for improvement of properties of epitaxial layers. Structure of reactor with induction heating is presented on Figure 1.

Method of solution

First of all we analyze spatio-temporal distribution of temperature. To analyze the distribution we determine the solution of the second Fourier law^[19]

$$c \frac{\partial T(r, \varphi, z, t)}{\partial t} = \text{div} \{ \lambda \cdot \text{grad} [T(r, \varphi, z, t)] \\ \vec{v}(r, \varphi, z, t) \cdot c(T) \cdot T(r, \varphi, z, t) \cdot C(r, \varphi, z, t) \} + \\ + p(r, \varphi, z, t), \quad (1)$$

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

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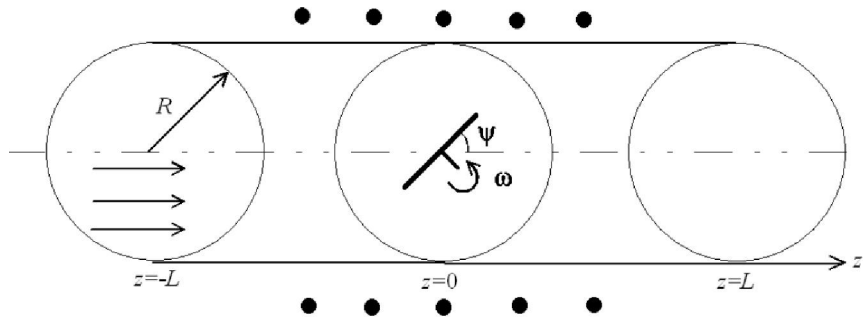


Figure 1a : Structure of reactor for gas phase epitaxy with sloping keeper of substrate

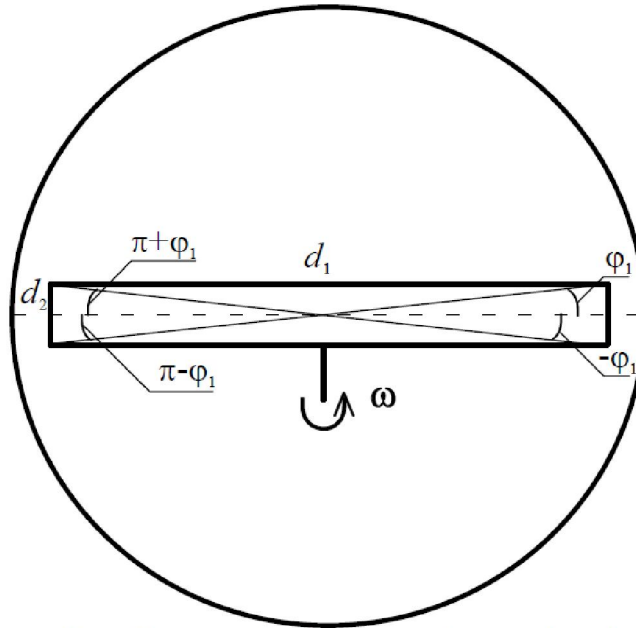


Figure 1b : View from side of keeper of substrate and approximation of the keeper by sloping lines with angle of sloping ϕ_1

ductivity could be determine by the following relation: $\lambda = \bar{v} \bar{l} c_v \rho / 3$, where \bar{v} is the speed of the gas molecules, \bar{l} is the average free path of gas molecules between collisions, c_v is the specific heat at constant volume, ρ is the density of gas.

To solve the Eq.(1) we shall to take into account moving of mixture of gases and concentration of the mixture. We determine speed of the moving and the concentration by solving the equation of Navier-Stokes and the second Fick's law, respectively. 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

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

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

where D is the diffusion coefficient of mixture of gases-reagents; 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 depositing on the substrate, flow is homogenous and one dimension. In this case boundary and initial conditions could be written as

$$\begin{aligned}
 C(r, \varphi, -L, t) = C_0, \quad C(r, -\varphi_1, z, t) = C(r, \varphi_1, z, t) = C(r, \pi - \varphi_1, z, t) = C(r, \pi + \varphi_1, z, t), \quad C(r, \varphi, z, 0) = \\
 C_0 \delta(z+L), \quad C(0, \varphi, z, t) \neq \infty, \quad C(r, \varphi, z, t)|_s = 0, \quad T(r, -\varphi_1, z, t) = T(r, \varphi_1, z, t) = T(r, \pi - \varphi_1, z, t) = \\
 T(r, \pi + \varphi_1, z, t), \quad \left. \frac{\partial C(r, \varphi, z, t)}{\partial r} \right|_{r=R} = 0, \quad -\lambda \left. \frac{\partial T(r, \varphi, z, t)}{\partial r} \right|_s = \sigma T^4(R, \varphi, z, t), \quad T(r, \varphi, z, 0) = \\
 = T_r, \quad \left. \frac{\partial T(r, \varphi, z, t)}{\partial \varphi} \right|_{\varphi=0} = \left. \frac{\partial T(r, \varphi, z, t)}{\partial \varphi} \right|_{\varphi=2\pi}, \quad -\lambda \left. \frac{\partial T(r, \varphi, z, t)}{\partial z} \right|_s = \sigma T^4(r, \varphi, -L, t), \quad (4)
 \end{aligned}$$

$$T(0, \varphi, z, t) \neq \infty, \quad \left. \frac{\partial v_r(r, \varphi, z, t)}{\partial r} \right|_{r=0} = 0, \quad \left. \frac{\partial v_r(r, \varphi, z, t)}{\partial r} \right|_{r=R} = 0, \quad v_r(r, -\varphi_1, z, t) = v_r(r, \varphi_1, z, t) =$$

$$\begin{aligned}
 v_r(r, \pi - \varphi_1, z, t) = v_r(r, \pi + \varphi_1, z, t), \quad v_\varphi(r, -\varphi_1, z, t) = v_\varphi(r, \varphi_1, z, t) = v_\varphi(r, \pi - \varphi_1, z, t) = v_\varphi(r, \pi + \varphi_1, z, t), \\
 v_z(r, -\varphi_1, z, t) = v_z(r, \varphi_1, z, t) = v_z(r, \pi - \varphi_1, z, t) = v_z(r, \pi + \varphi_1, z, t), \quad v_r(r, \varphi, -L, t) = 0, \quad v_r(r, \varphi, L, t) = 0, \\
 v_r(0, \varphi, z, t) \neq \infty, \quad v_z(r, \varphi, -L, t) = V_0, \quad v_z(r \pm d_2/2, \varphi, z \in [-d_2/2, d_2/2], 0) = \omega \cdot z \cdot \cos \psi \operatorname{tg}(\varphi_1), \\
 v_\varphi(r, \varphi, L, t) = 0, \quad v_\varphi(0, \varphi, z, t) \neq \infty, \quad v_z(r, \varphi, 0, t) = 0, \quad v_z(r, \varphi, L, t) = V_0, \quad v_z(r, \varphi, L, t) = V_0, \\
 v_z(0, \varphi, z, t) \neq \infty, \quad v_r(r, \varphi, z, 0) = 0, \quad v_\varphi(r, \varphi, z, 0) = 0,
 \end{aligned}$$

where $\sigma = 5,67 \cdot 10^{-8} \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-4}$, T_r is the room temperature, ω is the frequency of rotation of the substrate.

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

$$\begin{aligned}
 \frac{\partial v_r}{\partial t} = v \left\{ \frac{1}{r} \frac{\partial}{\partial r} \left[r \frac{\partial v_r(r, \varphi, z, t)}{\partial r} \right] + \frac{1}{r^2} \frac{\partial^2 v_r(r, \varphi, z, t)}{\partial \varphi^2} + \frac{\partial^2 v_r(r, \varphi, z, t)}{\partial z^2} \right\} - \\
 - v_r \frac{\partial v_r}{\partial r} - \frac{v_\varphi}{r} \frac{\partial v_\varphi}{\partial \varphi} - v_z \frac{\partial v_z}{\partial z} - \frac{\partial}{\partial r} \left(\frac{P}{\rho} \right) \quad (5a)
 \end{aligned}$$

$$\begin{aligned}
 \frac{\partial v_r}{\partial t} = v \left\{ \frac{1}{r} \frac{\partial}{\partial r} \left[r \frac{\partial v_\varphi(r, \varphi, z, t)}{\partial r} \right] + \frac{1}{r^2} \frac{\partial^2 v_\varphi(r, \varphi, z, t)}{\partial \varphi^2} + \frac{\partial^2 v_\varphi(r, \varphi, z, t)}{\partial z^2} \right\} - \\
 - v_r \frac{\partial v_r}{\partial r} - \frac{v_\varphi}{r} \frac{\partial v_\varphi}{\partial \varphi} - v_z \frac{\partial v_z}{\partial z} - \frac{1}{r} \frac{\partial}{\partial \varphi} \left(\frac{P}{\rho} \right) \quad (5b)
 \end{aligned}$$

$$\begin{aligned}
 \frac{\partial v_z}{\partial t} = v \left\{ \frac{1}{r} \frac{\partial}{\partial r} \left[r \frac{\partial v_z(r, \varphi, z, t)}{\partial r} \right] + \frac{1}{r^2} \frac{\partial^2 v_z(r, \varphi, z, t)}{\partial \varphi^2} + \frac{\partial^2 v_z(r, \varphi, z, t)}{\partial z^2} \right\} - \\
 - v_r \frac{\partial v_r}{\partial r} - \frac{v_\varphi}{r} \frac{\partial v_\varphi}{\partial \varphi} - v_z \frac{\partial v_z}{\partial z} - \frac{\partial}{\partial z} \left(\frac{P}{\rho} \right). \quad (5c)
 \end{aligned}$$

We determine solution of this system of equations by using of method of averaging of function correc-

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tions^[18-22]. Framework this approach first of all we determine the first-order approximation of components of speed of flow of mixture of gases. To determine the first-order approximation we replace of the required functions on their average values $v_r \rightarrow \alpha_{1r}$, $v_\varphi \rightarrow \alpha_{1\varphi}$, $v_z \rightarrow \alpha_{1z}$ in the right sides of equations of system (5). After the replacement and calculation required derivatives we obtain equations for the first-order approximations of the components

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

Integration of the left and the right sides on time of the relations (6) gives us possibility to obtain the first-order approximations of the components of speed of flow in the final form

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

The second-order approximations of components of speed of flow could be obtain by replacement of the required functions on the following sums $v_r \rightarrow \alpha_{2r} + v_{1r}$, $v_\varphi \rightarrow \alpha_{2\varphi} + v_{1\varphi}$, $v_z \rightarrow \alpha_{2z} + v_{1z}$. The average values α_{2r} , $\alpha_{2\varphi}$, α_{2z} are not yet known. Approximations for the components could be written as

$$\begin{aligned} \frac{\partial v_{2r}}{\partial t} = & v \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial v_{1r}}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_{1r}}{\partial \varphi^2} + \frac{\partial^2 v_{1r}}{\partial z^2} \right] - \frac{\partial}{\partial r} \left(\frac{P}{\rho} \right) - \\ & - (\alpha_{2r} + v_{1r}) \frac{\partial v_{1r}}{\partial r} - \frac{(\alpha_{2\varphi} + v_{1\varphi})}{r} \frac{\partial v_{1r}}{\partial \varphi} - (\alpha_{2z} + v_{1z}) \frac{\partial v_{1r}}{\partial z}, \end{aligned} \quad (8a)$$

$$\begin{aligned} \frac{\partial v_{2\varphi}}{\partial t} = & v \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial v_{1\varphi}}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_{1\varphi}}{\partial \varphi^2} + \frac{\partial^2 v_{1\varphi}}{\partial z^2} \right] - \frac{1}{r} \frac{\partial}{\partial \varphi} \left(\frac{P}{\rho} \right) - \\ & - (\alpha_{2r} + v_{1r}) \frac{\partial v_{1\varphi}}{\partial r} - \frac{(\alpha_{2\varphi} + v_{1\varphi})}{r} \frac{\partial v_{1\varphi}}{\partial \varphi} - (\alpha_{2z} + v_{1z}) \frac{\partial v_{1\varphi}}{\partial z}, \end{aligned} \quad (8b)$$

$$\begin{aligned} \frac{\partial v_{2z}}{\partial t} = & v \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial v_{1z}}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_{1z}}{\partial \varphi^2} + \frac{\partial^2 v_{1z}}{\partial z^2} \right] - \frac{\partial}{\partial z} \left(\frac{P}{\rho} \right) - \\ & - (\alpha_{2r} + v_{1r}) \frac{\partial v_{1z}}{\partial r} - \frac{(\alpha_{2\varphi} + v_{1\varphi})}{r} \frac{\partial v_{1z}}{\partial \varphi} - (\alpha_{2z} + v_{1z}) \frac{\partial v_{1z}}{\partial z}. \end{aligned} \quad (8c)$$

Integration of the above equations on time leads to the following result

$$\begin{aligned} v_{2r} = & v \int_0^t \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial v_{1r}}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_{1r}}{\partial \varphi^2} + \frac{\partial^2 v_{1r}}{\partial z^2} \right] d\tau - \frac{\partial}{\partial r} \left(\int_0^t \frac{P}{\rho} d\tau \right) - \\ & - \int_0^t (\alpha_{2r} + v_{1r}) \frac{\partial v_{1r}}{\partial r} d\tau - \int_0^t \frac{(\alpha_{2\varphi} + v_{1\varphi})}{r} \frac{\partial v_{1r}}{\partial \varphi} d\tau - \int_0^t (\alpha_{2z} + v_{1z}) \frac{\partial v_{1r}}{\partial z} d\tau, \end{aligned} \quad (8d)$$

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

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

$$v_{2z} = V_0 + v \int_0^t \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial v_{1z}}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_{1z}}{\partial \varphi^2} + \frac{\partial^2 v_{1z}}{\partial z^2} \right] d\tau - \frac{\partial}{\partial z} \left(\int_0^t \frac{P}{\rho} d\tau \right) -$$

$$- \int_0^t (\alpha_{2r} + v_{1r}) \frac{\partial v_{1z}}{\partial r} d\tau - \int_0^t \frac{(\alpha_{2\varphi} + v_{1\varphi})}{r} \frac{\partial v_{1z}}{\partial \varphi} d\tau - \int_0^t (\alpha_{2z} + v_{1z}) \frac{\partial v_{1z}}{\partial z} d\tau. \quad (8f)$$

Farther we determine average values α_{2r} , $\alpha_{2\varphi}$, α_{2z} . The average values have been calculated by the following relations^[18-22]

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

$$\alpha_{2\varphi} = \frac{1}{\pi \Theta R^2 L} \int_0^{\Theta R} \int_0^{2\pi} \int_{-L}^L (v_{2\varphi} - v_{1\varphi}) dz d\varphi dr dt \quad (9)$$

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

where Θ is the continuance of moving of mixture of gases through considered horizontal 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

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

$$\text{where } A_1 = 1 + \int_0^{\Theta} (\Theta - t) \int_0^R \int_0^{2\pi} \int_{-L}^L \frac{\partial v_{1r}}{\partial r} dz d\varphi dr dt, \quad B_1 = \int_0^{\Theta} (\Theta - t) \int_0^R \int_0^{2\pi} \int_{-L}^L \frac{\partial v_{1r}}{\partial \varphi} dz d\varphi dr dt,$$

$$C_1 = C_2 = \frac{\pi}{2} \Theta^2 R^2 V_0, \quad D_1 = v \int_0^{\Theta} \int_0^R \int_0^{2\pi} \int_{-L}^L \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial v_{1r}}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_{1r}}{\partial \varphi^2} + \frac{\partial^2 v_{1r}}{\partial z^2} \right] dz d\varphi dr (\Theta -$$

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

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

Solution of the above system of equations could be determined by standard approaches^[23] and could be written as

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

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

In this section we obtained 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 rewrite Eqs.(1) and (3) by using cylindrical system of coordinate

$$\begin{aligned}
 c \frac{\partial T(r, \varphi, z, t)}{\partial t} &= \lambda \frac{\partial^2 T(r, \varphi, z, t)}{\partial r^2} + \frac{\lambda}{r^2} \frac{\partial^2 T(r, \varphi, z, t)}{\partial \varphi^2} + \lambda \frac{\partial^2 T(r, \varphi, z, t)}{\partial z^2} - \\
 &- c \cdot \frac{\partial}{\partial r} [v_r(r, \varphi, z, t) \cdot C(r, \varphi, z, t) \cdot T(r, \varphi, z, t)] - \frac{c}{r} \frac{\partial}{\partial \varphi} [v_\varphi(r, \varphi, z, t) \cdot C(r, \varphi, z, t) \cdot \\
 &\cdot T(r, \varphi, z, t)] - c \cdot \frac{\partial}{\partial z} [v_z(r, \varphi, z, t) \cdot C(r, \varphi, z, t) \cdot T(r, \varphi, z, t)] + p(r, \varphi, z, t), \quad (12)
 \end{aligned}$$

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

$$\begin{aligned}
& + \frac{1}{r^2} \frac{\partial}{\partial \varphi} \left[D \frac{\partial C(r, \varphi, z, t)}{\partial \varphi} \right] - \frac{1}{r} \frac{\partial}{\partial \varphi} \left[C(r, \varphi, z, t) v_\varphi(r, \varphi, z, t) \right] + \\
& + \frac{\partial}{\partial z} \left[D \frac{\partial C(r, \varphi, z, t)}{\partial z} \right] - \frac{\partial}{\partial z} \left[C(r, \varphi, z, t) v_z(r, \varphi, z, t) \right].
\end{aligned} \tag{13}$$

In this section we calculate components of speed of gas-reagents, which are used to growth an epitaxial layer, and gas-carrier as the second-order approximations framework method of averaging of function corrections. Usually the second-order approximation is enough good approximation to make qualitative analysis and obtain some quantitative results. Results of analytical calculation have been checked by comparison with results of numerical simulation.

To determine spatio-temporal distributions 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_{IT} and α_{IC} in right sides of the above equations. Farther we used recently considered algorithm to obtain the first-order approximations of temperature and concentration of gas-reagents

$$\begin{aligned}
T_1(r, \varphi, z, t) = & T_r + \int_0^t \frac{p(r, \varphi, z, \tau)}{c} d\tau - \alpha_{IT} \alpha_{IC} \int_0^t \frac{\partial v_r(r, \varphi, z, \tau)}{\partial r} d\tau - \\
& - \frac{\alpha_{IT} \alpha_{IC}}{r} \int_0^t \frac{\partial v_\varphi(r, \varphi, z, \tau)}{\partial \varphi} d\tau - \alpha_{IT} \alpha_{IC} \int_0^t \frac{\partial v_z(r, \varphi, z, \tau)}{\partial z} d\tau,
\end{aligned} \tag{14}$$

$$\begin{aligned}
C_1(r, \varphi, z, t) = & -\alpha_{IT} \alpha_{IC} \int_0^t \frac{\partial v_r(r, \varphi, z, \tau)}{\partial r} d\tau - \frac{\alpha_{IC}}{r} \int_0^t \frac{\partial [r v_r(r, \varphi, z, \tau)]}{\partial r} d\tau - \\
& - \frac{\alpha_{IC}}{r} \int_0^t \frac{\partial v_\varphi(r, \varphi, z, \tau)}{\partial \varphi} d\tau - \alpha_{IC} \int_0^t \frac{\partial v_z(r, \varphi, z, \tau)}{\partial z} d\tau.
\end{aligned} \tag{15}$$

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

$$\begin{aligned}
\alpha_{IT} = & \frac{1}{\pi \Theta R^2 L} \int_0^\Theta \int_0^R \int_0^{2\pi} \int_0^L T_1(r, \varphi, z, \tau) dz d\varphi dr dt, \\
\alpha_{IC} = & \frac{1}{\pi \Theta R^2 L} \int_0^\Theta \int_0^R \int_0^{2\pi} \int_0^L C_1(r, \varphi, z, \tau) dz d\varphi dr dt,
\end{aligned} \tag{16}$$

Substitution of the first-order approximations of temperature and concentration of gas mixer into relations (16) gives us the following results^[23]

$$\begin{aligned}
\alpha_{IC} = & C_0 / L \cdot \left[1 + \frac{1}{\pi \Theta R L} \int_0^\Theta (\Theta - t) \int_0^R \int_0^{2\pi} \int_0^L v_r(R, \varphi, z, t) dz d\varphi dt + \frac{\Theta V_0}{R L} \right], \\
\alpha_{IT} = & \left[T_r + \frac{1}{\pi \Theta R^2 L} \int_0^\Theta (\Theta - t) \int_0^R \int_0^{2\pi} \int_0^L \frac{p(r, \varphi, z, t)}{c} dz d\varphi dr dt \right] \left\{ 1 + \frac{C_0}{\pi \Theta R L^2} \int_0^\Theta (\Theta - t) \times \right.
\end{aligned}$$

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

The second-order approximations of temperature and concentration of gases- reagents we determine framework the method of averaging of function corrections^[16-21], i.e. by replacement of the required functions in right sides of equations (12) and (13) on the following sums $T \rightarrow \alpha_{2T} + T_1$, $C \rightarrow \alpha_{2C} + C_1$. In this case the second-order approximations of the above required functions could be written as

$$\begin{aligned} c \cdot T_2(r, \varphi, z, t) = & \lambda \int_0^t \frac{\partial^2 T_1(r, \varphi, z, \tau)}{\partial r^2} d\tau + \lambda \frac{1}{r^2} \int_0^t \frac{\partial^2 T_1(r, \varphi, z, \tau)}{\partial \varphi^2} d\tau + \lambda \int_0^t \frac{\partial^2 T_1(r, \varphi, z, \tau)}{\partial z^2} d\tau + \\ & + \int_0^t p(r, \varphi, z, \tau) d\tau - c \cdot \frac{\partial}{\partial r_0} \int_0^t \{v_r(r, \varphi, z, \tau) \cdot [\alpha_{2C} + C_1(r, \varphi, z, \tau)] \cdot [\alpha_{2T} + T_1(r, \varphi, z, \tau)]\} d\tau + \\ & + T_r - \frac{c}{r} \frac{\partial}{\partial \varphi_0} \int_0^t \{v_\varphi(r, \varphi, z, \tau) \cdot [\alpha_{2C} + C_1(r, \varphi, z, \tau)] \cdot [\alpha_{2T} + T_1(r, \varphi, z, \tau)]\} d\tau - \\ & - c \cdot \frac{\partial}{\partial z_0} \int_0^t \{v_z(r, \varphi, z, \tau) \cdot [\alpha_{2C} + C_1(r, \varphi, z, \tau)] \cdot [\alpha_{2T} + T_1(r, \varphi, z, \tau)]\} d\tau, \end{aligned} \quad (17)$$

$$\begin{aligned} C_2(r, \varphi, z, t) = & \frac{1}{r} \frac{\partial}{\partial r_0} \int_0^t r D \frac{\partial C_1(r, \varphi, z, \tau)}{\partial r} d\tau + \frac{1}{r^2} \frac{\partial}{\partial \varphi_0} \int_0^t D \frac{\partial C_1(r, \varphi, z, \tau)}{\partial \varphi} d\tau + \frac{\partial}{\partial z_0} \int_0^t D \times \\ & \times \frac{\partial C_1(r, \varphi, z, \tau)}{\partial z} d\tau - \frac{1}{r} \frac{\partial}{\partial r} \left\{ r \int_0^t [\alpha_{2C} + C_1(r, \varphi, z, \tau)] \cdot v_r(r, \varphi, z, \tau) d\tau \right\} - \frac{1}{r} \frac{\partial}{\partial \varphi_0} \int_0^t v_\varphi(r, \varphi, z, \tau) \cdot \\ & \cdot [\alpha_{2C} + C_1(r, \varphi, z, \tau)] d\tau - \frac{\partial}{\partial z_0} \int_0^t [\alpha_{2C} + C_1(r, \varphi, z, \tau)] \cdot v_z(r, \varphi, z, \tau) d\tau + C_0 \delta(z + L). \end{aligned} \quad (18)$$

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

$$\begin{aligned} \alpha_{2T} = & \frac{1}{\pi \Theta R^2 L} \int_0^\Theta \int_0^{2\pi} \int_{-L}^L r \int_0^t (T_2 - T_1) dz d\varphi dr dt, \\ \alpha_{2C} = & \frac{1}{\pi \Theta R^2 L} \int_0^\Theta \int_0^{2\pi} \int_{-L}^L r \int_0^t (C_2 - C_1) dz d\varphi dr dt. \end{aligned} \quad (19)$$

Substitution of the first- and the second-order approximations of temperature and concentration of mixture into relations (19) gives us possibility to obtain equations to determine required average values

$$\begin{aligned} \alpha_{2T} = & \left(\frac{\lambda \sigma}{c \pi \Theta R L} \int_0^\Theta (\Theta - t) \int_0^{2\pi} \int_{-L}^L T^4(R, \varphi, z, t) dz d\varphi dt - \int_0^\Theta (\Theta - t) \int_0^{2\pi} \int_{-L}^L T_1(R, \varphi, z, t) dz d\varphi dt \times \right. \\ & \times \frac{\lambda}{c \pi \Theta R^2 L} + \frac{\lambda}{c \pi \Theta R^2 L} \int_0^\Theta (\Theta - t) \int_0^{2\pi} \int_{-L}^L T_1(0, \varphi, z, t) dz d\varphi dt - \int_0^\Theta (\Theta - t) \int_0^{2\pi} \int_{-L}^L v_r(R, \varphi, z, t) \times \end{aligned}$$

$$\begin{aligned}
& \times \left\{ [\alpha_{2C} + C_1(R, \varphi, z, t)] T_1(R, \varphi, z, t) - \alpha_{1T} \alpha_{1C} \right\} dz d\varphi dt \frac{1}{\pi \Theta R L} - \frac{1}{\pi \Theta R^2 L} \int_0^\Theta (\Theta - t) \times \\
& \times \int_0^R \int_{-L}^L v_r(r, \varphi, z, \tau) \{ T_1(r, \varphi, z, t) [\alpha_{2C} + C_1(r, \varphi, z, t)] - \alpha_{1T} \alpha_{1C} \} dz d\varphi r dr dt - \frac{V_0}{\pi \Theta R^2 L} \times \\
& \times \int_0^\Theta (\Theta - t) \int_0^R \int_0^{2\pi} [(\alpha_{2C} + C_0) \cdot T_1(r, \varphi, L, t) - \alpha_{1T} \alpha_{1C}] d\varphi dr dt \left\{ 1 + \frac{1}{\pi \Theta R L} \int_0^\Theta \int_0^{2\pi} \int_{-L}^L v_r(R, \varphi, z, t) \times \right. \\
& \times [\alpha_{2C} + C_1(R, \varphi, z, t)] dz d\varphi (\Theta - t) dt - \frac{1}{\pi \Theta R^2 L} \int_0^\Theta (\Theta - t) \int_0^R \int_0^{2\pi} \int_{-L}^L [\alpha_{2C} + C_1(r, \varphi, z, t)] \times \\
& \left. \times v_r(r, \varphi, z, \tau) dz d\varphi r dr dt + 2V_0(\alpha_{2C} + C_0) \frac{\Theta}{L} \right\}^{-1}, \\
\alpha_{2C} &= \frac{1}{\pi \Theta R^2 L} \int_0^\Theta (\Theta - t) \int_0^R \int_0^{2\pi} D \left[\frac{\partial C_1(r, \varphi, z, \tau)}{\partial z} \Big|_{z=L} - \frac{\partial C_1(r, \varphi, z, \tau)}{\partial z} \Big|_{z=-L} \right] d\varphi dr dt - \\
& - \frac{1}{\pi \Theta R^2 L} \int_0^\Theta (\Theta - t) \int_0^{2\pi} \int_{-L}^L \{ r [\alpha_{2C} - \alpha_{1C} + C_1(R, \varphi, z, \tau)] \cdot v_r(R, \varphi, z, \tau) \} dz d\varphi dt - \\
& - \frac{V_0}{\pi \Theta R^2 L} \int_0^\Theta (\Theta - t) \int_0^R \int_0^{2\pi} (\alpha_{2C} - \alpha_{1C} + C_0) dz d\varphi r dr dt.
\end{aligned}$$

DISCUSSION

In this section we analyzed dynamics of mass and heat transport during growth of films in reactors for gas phase epitaxy to determine conditions for improvement of growth of epitaxial layers. Figure 2a shows dependence of concentration of material of epitaxial layer on frequency of rotation of substrate ω in a horizontal reactor (curve 2) in comparison with analogous dependence for vertical reactor (curve 1). Curve 3 on Figure 2a corresponds to average value of sloping angle (i.e. $\psi = 45^\circ$) of keeper of substrate in comparison with direction of flow gazes. Figure 2b shows comparison of frequency dependences of concentration of gas-reagents at atmospheric pressure and smaller in ten times pressure (curves 1 and 2, respectively). Figure 3a shows dependences of concentration of materials of epitaxial layer on diffusion coefficient D in vertical and horizontal reactors (curves 1 and 2, respectively). Curve 3 on Figure 2a corresponds to average value of sloping angle (i.e. $\psi = 45^\circ$) of keeper of substrate in comparison with direction of flow gazes. Figure 3b shows comparison of dependences of concentration of gas-reagents on diffusion coefficient at atmospheric pressure and smaller in ten times pressure (curves 1 and 2, respectively). Increasing of diffusion coefficient leads to increasing of speed of flow of gases. In this situation one can find decreasing growth rate of epitaxial layers. Value of dopant diffusion coefficient could be increased by increasing of temperature of growth. Dependences of concentration of gases-reagents on kinematical viscosity ν are presented on Figure 4a for vertical and horizontal reactors (curves 1 and 2,

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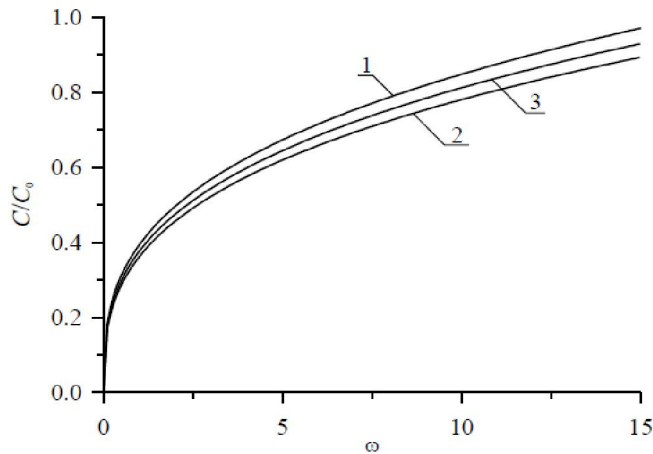


Figure 2a : Dependence of concentration of mixture of gases on frequency of rotation of substrate ω . curve 1 corresponds to vertical reactor, curve 2 corresponds to horizontal reactor, curve 3 corresponds to average value of sloping angle (i.e. $\psi = 45^\circ$) of keeper of substrate in comparison with direction of flow gases

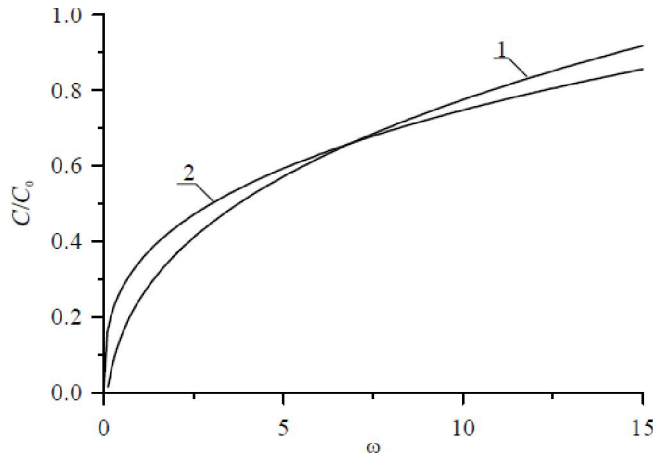


Figure 2b : Dependence of concentration of mixture of gases on frequency of rotation of substrate ω , curve 1 corresponds to atmospheric pressure, curve 2 corresponds to smaller pressure

respectively). Curve 3 on Figure 4a corresponds to average value of sloping angle (i.e. $\psi = 45^\circ$) of keeper of substrate in comparison with direction of flow gases. The Figure 4b shows comparison of dependences of concentration of gas-reagents on kinematical viscosity at atmospheric pressure and smaller in ten times pressure (curves 1 and 2, respectively). Reason of decreasing of concentration of gas-reagents with increasing of kinematical viscosity is decreasing of speed of transport of the gases. Dependences of concentration of gas-reagents on speed of flow on inlet of reaction zone V_0 are shown on Figure 5a for vertical and horizontal re-

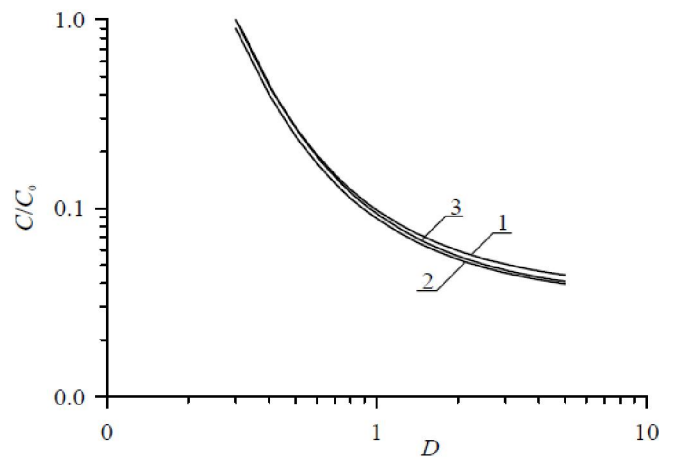


Figure 3a : Dependence of concentration of mixture of gases on diffusion coefficient D . Curve 1 corresponds to vertical reactor. Curve 2 corresponds to horizontal reactor. Curve 3 corresponds to average value of sloping angle (i.e. $\psi = 45^\circ$) of keeper of substrate in comparison with direction of flow gases

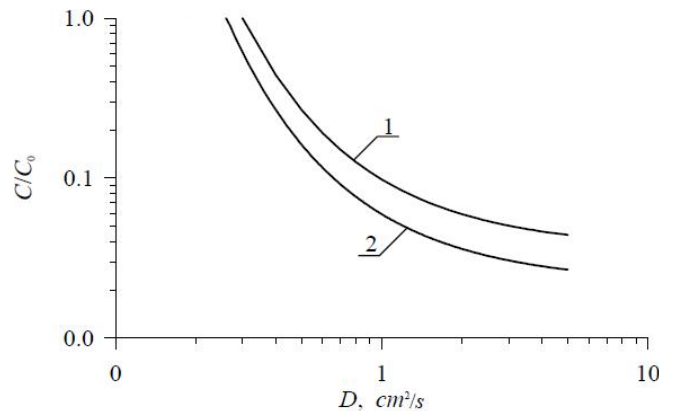


Figure 3b : Dependence of concentration of mixture of gases on diffusion coefficient D . Curve 1 corresponds to atmospheric pressure. Curve 2 corresponds to smaller pressure

actors (curves 1 and 2, respectively). Curve 3 on Figure 5a corresponds to average value of sloping angle (i.e. $\psi = 45^\circ$) of keeper of substrate in comparison with direction of flow gases. The Figure 5b shows comparison of dependences of concentration of gas-reagents on speed of flow on inlet of reaction zone at atmospheric pressure and smaller in ten times pressure (curves 1 and 2, respectively). Changing of angle ψ leads to negligible quantitative changing of dependences of concentration of gas-reagents with the same qualitative structure of curves.

It is known (see, for example,^[24]), that increasing of temperature of reaction zone leads to activation of chemical reaction during growth of

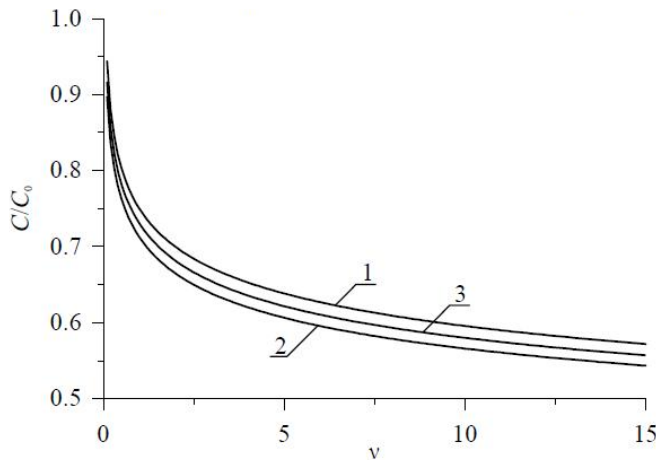


Figure 4a : Dependence of concentration of mixture of gases on viscosity ν . Curve 1 corresponds to vertical reactor. Curve 2 corresponds to horizontal reactor. Curve 3 corresponds to average value of sloping angle (i.e. $\psi = 45^\circ$) of keeper of substrate in comparison with direction of flow gazes

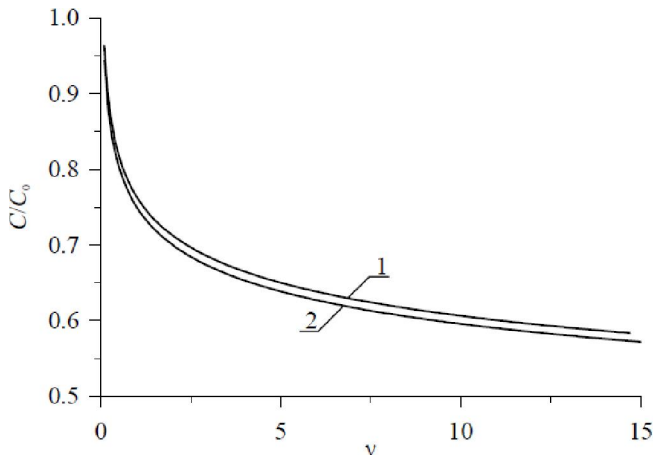


Figure 4b : Dependence of concentration of mixture of gases on viscosity ν . Curve 1 corresponds to atmospheric pressure, curve 2 corresponds to smaller pressure

epitaxial layer. In this situation growth rate of the epitaxial layer increases. At the same time surficial diffusion of material of epitaxial layer accelerates. In this situation homogeneity of surface of the epitaxial layer increases. However one can find losing of heat during convective heat exchange from surface of the system keeper of substrate - substrate^[16]. To compensate the losing it is attracting an interest choosing of power of induction heating of reaction zone. In this situation relaxation time of heating ϑ could be estimated framework recently introduced approach^[25] and approximately equal $\vartheta \approx (6\pi - 1)R^2 / 24\lambda_0$, where λ_0 is the average value of heat conduction coefficient. For stationary regime of heating

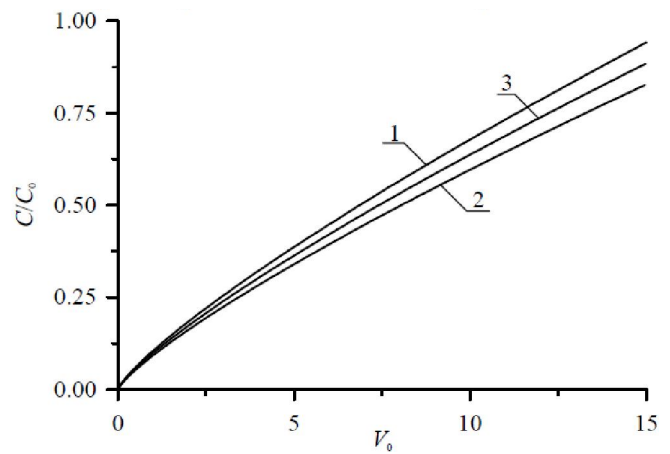


Figure 5a : Dependence of concentration of mixture of gases on inlet velocity V_0 , curve 1 corresponds to vertical reactor. curve 2 corresponds to horizontal reactor. curve 3 corresponds to average value of sloping angle (i.e. $\psi = 45^\circ$) of keeper of substrate in comparison with direction of flow gazes

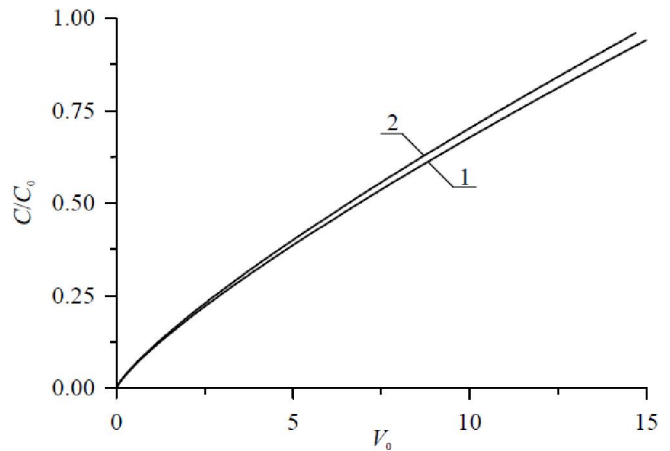


Figure 5b : Dependence of concentration of mixture of gases on inlet velocity V_0 , curve 1 corresponds to atmospheric pressure, curve 2 corresponds to smaller pressure

power of induction heating to compensate losing of heat convective heat exchange could be estimated by using the following relation:

$$\int_0^R r \cdot p(r, \varphi, z, t) dr \approx \approx \sigma \cdot T^4(R, \varphi, z, t) + \Theta \cdot v_z(R, \varphi, z, t) / 4\pi LR^2 \text{ [16]}$$

CONCLUSION

In this paper we analyzed dynamics of mass and heat transport in reactors for gas phase epitaxy. Are have been formulated several recommendations to

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improve properties of epitaxial layers for vertical and horizontal reactors and reactors with spooled keepers of substrates.

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