

Nano Science and Nano Technology

An Indian Journal

Full Paper

NSNTAJ, 9(6), 2015 [215-226]

On controlling of gas and heat transport in a vertical reactor process to improve properties of epitaxial layers

E.L.Pankratov^{1*}, E.A.Bulaeva^{1,2}

¹Nizhny Novgorod State University, 23 Gagarin avenue, Nizhny Novgorod, 603950, (RUSSIA)

²Nizhny Novgorod State University of Architecture and Civil Engineering, 65 Il'insky street, Nizhny Novgorod, 603950, (RUSSIA)

E-mail: elp2004@mail.ru

ABSTRACT

In this paper we analyzed mass and heat transport in a reactor from gas phase during growth an epitaxial layer. Based on results of the analysis we analyzed dependences of properties of grown layers on parameters of technological process. © 2015 Trade Science Inc. - INDIA

KEYWORDS

Gaz phase epitaxy;
Prognosis of epitaxy;
Epitaxial layer improvement.

INTRODUCTION

Development of solid state electronics and wide using heterostructures for manufacturing the electronic devices leads to necessity to improve properties of these devices. To manufacture a heterostructure it could be used different approaches: molecular-beam epitaxy, epitaxy from gas phase, magnetron sputtering. Manufacturing and using heterostructures have been described in large number of works^[1-14]. They are many experimental results have been obtain and reported in literature. It has been investigated dynamics of growth of epitaxial layers on parameters of technological (temperature of growth, pressure of grown materials et al) and physical (diffusion coefficient, viscosity et al) processes. They are have been obtained recommendations to improve properties of epitaxial layers, decreasing of losing of using for epitaxy materials (for example, some part of materials will be loosed through gap between keeper of substrate and external casing), decreasing of energy cost. How-

ever mathematical modeling of physical (including technological) processes gives a possibility to decrease cost of investigation of possibility to improve technological process. Necessity using mathematical modeling leads to development approaches to solve equations. Usually numerical approaches are developing and/or using in literature^[10,13]. Framework the present paper is development of analytical approach for analysis of mass and heat transport in a reactor for gas phase to obtain dependences of properties epitaxial layers on parameters of technological process. Analytical approaches give a possibility to analyze processes more demonstrative. Main aims of our paper are development of analytical approaches to analyze technological processes and formulation recommendations to improve properties of epitaxial layers.

Method of solution

In this paper we consider vertical reactor for epitaxy from gas phase (see Figure 1). The reactor consist of an external casing, a keeper of substrate

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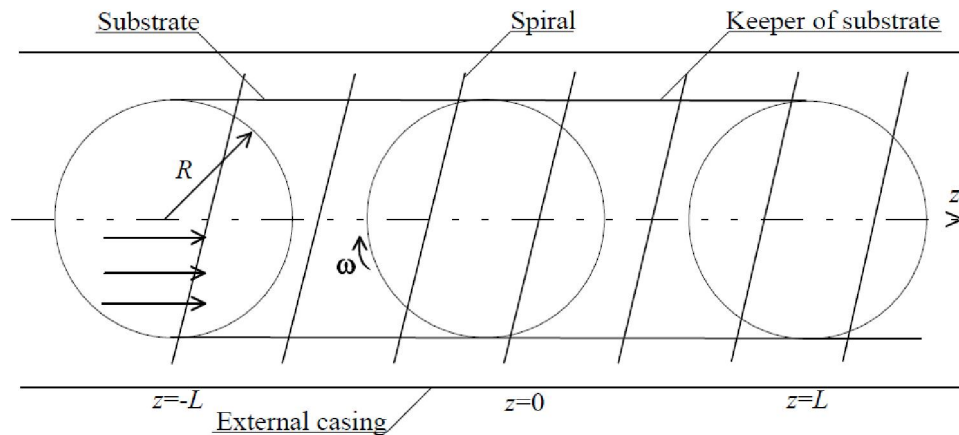


Figure 1 : A reactor for the gas phase epitaxy in neighborhoods of reaction zone $z \in [-L, L]$, Here z is the coordinate along reactor axis, R is the radius of keeper of substrate, ω is the frequency of rotation of keeper of substrate

with a substrate and a spiral around the casing in area of growth of an epitaxial layer to obtain induction heating for atomization chemical reaction. In inlet of reaction area mixture of gas-reagents supplied together with a gas-carrier. Main aim of the present paper is development of analytical approach for analysis and analysis of dependences of properties of epitaxial layer on parameters of technological processes.

First of all we analyze spatio-temporal distribution of temperature. To analyze the distribution we determine the solution of the second Fourier law^[15]

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

where \vec{v} is the speed of flow of mixture of gases-reagents; 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 conductivity 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

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

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

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

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

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

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

$$\left. \frac{\partial v_r(r, \varphi, z, t)}{\partial r} \right|_{r=0} = \left. \frac{\partial v_r(r, \varphi, z, t)}{\partial r} \right|_{r=R}, \left. \frac{\partial v_\varphi(r, \varphi, z, t)}{\partial \varphi} \right|_{\varphi=0} = \left. \frac{\partial v_\varphi(r, \varphi, z, t)}{\partial \varphi} \right|_{\varphi=2\pi},$$

$$\left. \frac{\partial v_r(r, \varphi, z, t)}{\partial r} \right|_{r=0} = \left. \frac{\partial v_r(r, \varphi, z, t)}{\partial r} \right|_{r=R}, \left. \frac{\partial v_\varphi(r, \varphi, z, t)}{\partial \varphi} \right|_{\varphi=0} = \left. \frac{\partial v_\varphi(r, \varphi, z, t)}{\partial \varphi} \right|_{\varphi=2\pi}, \quad (4)$$

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

$$v_r(r, 0, z, t) = v_r(r, 2\pi, z, t), v_r(0, \varphi, z, t) \neq \infty, v_\varphi(r, \varphi, 0, t) = \omega r, v_\varphi(r, \varphi, -L, t) = 0, v_\varphi(r, \varphi, L, t) = 0, \\ v_\varphi(r, 0, z, t) = v_\varphi(r, 2\pi, z, t), v_\varphi(0, \varphi, z, t) \neq \infty, v_z(r, \varphi, -L, t) = V_0, v_z(r, \varphi, 0, t) = 0, v_z(r, \varphi, L, t) = 0, \\ v_z(r, 0, z, t) = v_z(r, 2\pi, z, t), v_z(0, \varphi, z, t) \neq \infty, v_r(r, \varphi, z, 0) = 0, v_\varphi(r, \varphi, z, 0) = 0, v_z(r, \varphi, -L, 0) = V_0,$$

where $\sigma = 5.67 \cdot 10^{-8} \text{ W} \cdot \text{m}^{-2} \cdot \text{K}^{-4}$, 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

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

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

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

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$$-v_r \frac{\partial v_r}{\partial r} - \frac{v_\varphi}{r} \frac{\partial v_\varphi}{\partial \varphi} - v_z \frac{\partial v_z}{\partial z} - \frac{\partial}{\partial z} \left(\frac{P}{\rho} \right). \quad (5c)$$

We determine solution of this system of equations by using of method of averaging of function corrections^[16-22]. 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

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

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

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

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

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

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

Farther we determine average values α_{2r} , $\alpha_{2\varphi}$, α_{2z} . The average values have been calculated by the following relations^[17-22]

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

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

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

where Θ is the continuance of moving of mixture of gases through 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 $A_1 = 1 + \int_0^{\Theta} (\Theta - t) \int_0^R \int_0^{2\pi} \int_{-L}^L \frac{\partial v_{1r}}{\partial r} dz d\varphi dr dt$, $B_1 = \int_0^{\Theta} (\Theta - t) \int_0^{R2\pi} \int_{-L}^L \frac{\partial v_{1r}}{\partial \varphi} dz d\varphi dr dt$,

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

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$$\begin{aligned}
 & -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 \\
 & \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^[24] 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

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

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

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_{1T} and α_{1C} 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 mixer

$$\begin{aligned}
T_1(r, \varphi, z, t) &= T_r + \int_0^t \frac{p(r, \varphi, z, \tau)}{c} d\tau - \alpha_{1T} \alpha_{1C} \int_0^t \frac{\partial v_r(r, \varphi, z, \tau)}{\partial r} d\tau - \\
&- \frac{\alpha_{1T} \alpha_{1C}}{r} \int_0^t \frac{\partial v_\varphi(r, \varphi, z, \tau)}{\partial \varphi} d\tau - \alpha_{1T} \alpha_{1C} \int_0^t \frac{\partial v_z(r, \varphi, z, \tau)}{\partial z} d\tau,
\end{aligned} \tag{14}$$

$$\begin{aligned}
C_1(r, \varphi, z, t) &= -\alpha_{1T} \alpha_{1C} \int_0^t \frac{\partial v_r(r, \varphi, z, \tau)}{\partial r} d\tau - \frac{\alpha_{1C}}{r} \int_0^t \frac{\partial [r v_r(r, \varphi, z, \tau)]}{\partial r} d\tau - \\
&- \frac{\alpha_{1C}}{r} \int_0^t \frac{\partial v_\varphi(r, \varphi, z, \tau)}{\partial \varphi} d\tau - \alpha_{1C} \int_0^t \frac{\partial v_z(r, \varphi, z, \tau)}{\partial z} d\tau.
\end{aligned} \tag{15}$$

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

$$\begin{aligned}
\alpha_{1T} &= \frac{1}{\pi \Theta R^2 L} \int_0^\Theta \int_0^R \int_0^{2\pi} \int_0^L T_1(r, \varphi, z, \tau) d z d \varphi d r d t, \\
\alpha_{1C} &= \frac{1}{\pi \Theta R^2 L} \int_0^\Theta \int_0^R \int_0^{2\pi} \int_0^L C_1(r, \varphi, z, \tau) d z d \varphi d r d t.
\end{aligned} \tag{16}$$

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

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

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

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

The second-order approximations of temperature and concentration of mixture of gases we determine framework the method of averaging of function corrections^[16-23], 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

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

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

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

$$- c \cdot \frac{\partial}{\partial z} \int_0^t \{v_z(r, \varphi, z, \tau) \cdot [\alpha_{2C} + C_1(r, \varphi, z, \tau)] \cdot [\alpha_{2T} + T_1(r, \varphi, z, \tau)]\} d\tau, \quad (18)$$

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

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

$$\cdot [\alpha_{2C} + C_1(r, \varphi, z, \tau)] d\tau - \frac{\partial}{\partial z} \int_0^t [\alpha_{2C} + C_1(r, \varphi, z, \tau)] \cdot v_z(r, \varphi, z, \tau) d\tau + C_0 \delta(z + L). \quad (19)$$

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

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

$$\alpha_{2C} = \frac{1}{\pi \Theta R^2 L} \int_0^\Theta \int_0^{2\pi} \int_{-L}^L (C_2 - C_1) dz d\varphi dr dt. \quad (20)$$

Substitution of the first- and the second-order approximations of temperature and concentration of mixture into relations (20) 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 \\
& \times \{ [\alpha_{2C} + C_1(R, \varphi, z, t)] T_1(R, \varphi, z, t) - \alpha_{1T} \alpha_{1C} \} 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/2} \int_0^{2\pi} \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 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 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 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 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 r \int_0^{2\pi} (\alpha_{2C} - \alpha_{1C} + C_0) dz d\varphi dr dt.
\end{aligned}$$

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 improve properties of epitaxial layers. Figure 2 shows dependence of concentration of material of epitaxial layer on frequency of rotation of substrate. The figure 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 dependence of concentration of material of epitaxial layer on diffusion coefficient D . 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

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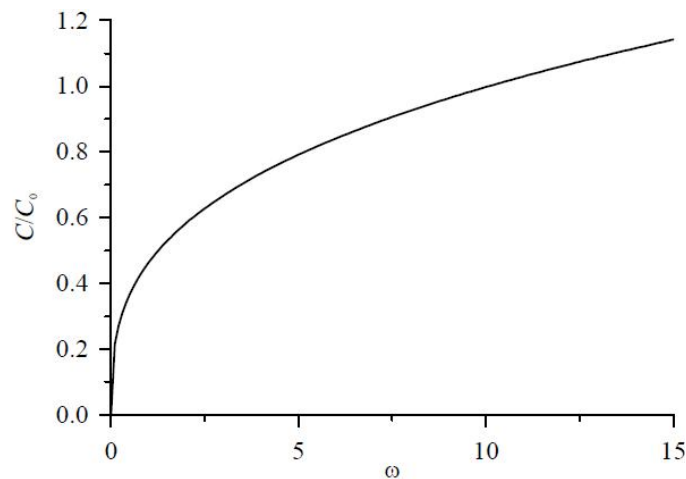


Figure 2 : Dependence of concentration of mixture of gases on frequency of rotation of substrate

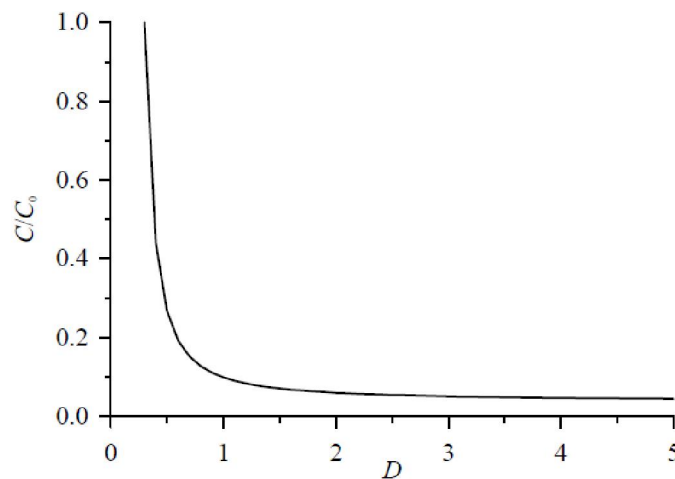


Figure 3 : Dependence of concentration of mixture of gases on diffusion coefficient

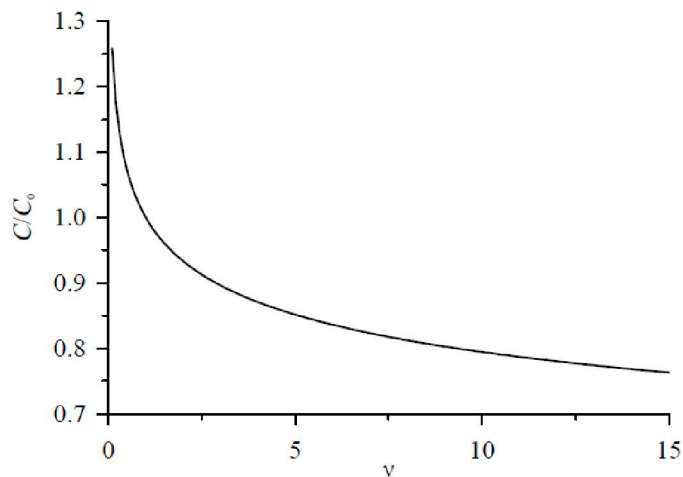


Figure 4 : Dependence of concentration of mixture of gases on kinematical viscosity ν

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. 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.

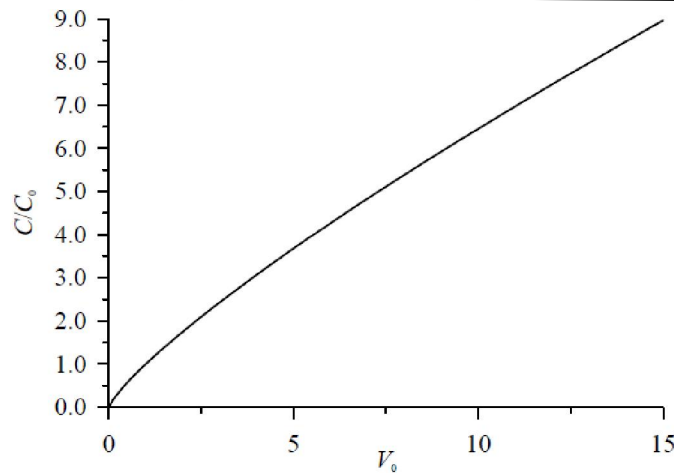


Figure 5 : Dependence of concentration of mixture of gases on inlet speed

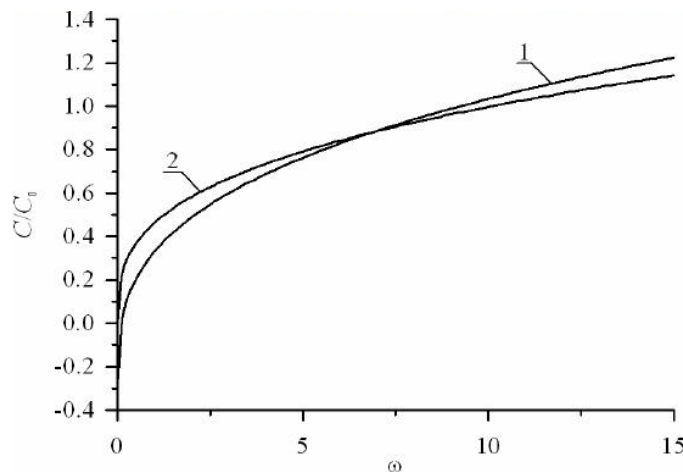


Figure 6 : Dependences of concentration of mixture of gases on frequency of rotation of substrate for approximately atmospheric pressure of gases in the reactor (curve 1) and to decreased into ten time pressure of gases (curve 2)

Increasing of speed V_0 leads to increasing of concentration of reagents in reaction zone and to increasing of speed of growth of epitaxial layers.

The Figure 6 shows comparison of dependences of concentration of mixture of gases of reagents on frequency of rotation of substrate for different values of pressure in reactors. Curve 1 corresponds to approximately atmospheric pressure of gases in the reactor (value of pressure at the reactor outlet is atmospheric P_{atm} , value of pressure at the reactor inlet is atmospheric $1.2P_{atm}$). Curve 2 corresponds to decreased into ten time pressure of gases. The figure shows, that decreasing of pressure in reactor gives us possibility to decrease inertness of processes.

It should be noted, that it is attracted an interest choosing of value of power of induction heating of growth area to compensate heat loss due to convec-

tive heat^[22]. In this case time of heating of reactor zone \mathcal{G} could be estimated framework recently introduced approach^[23] and could be calculated as $\mathcal{G} \approx (6\pi - 1)R^2/24\lambda_0$, 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:

$$\int_0^R r \cdot p(r, \varphi, z, t) dr \approx \sigma \cdot T^4(R, \varphi, z, t) + \Theta \times$$

$$\times v_z(R, \varphi, z, t)/4\pi LR^2 .$$

It should be also noted, that all results, presented in Figs. 2-6, have been calculated by using method of averaging of function corrections. Our several recent analytical results have been compared with numerical and experimental one. After the comparison we obtain deference

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between analytical and numerical/ experimental results framework several percents or few their decades.

CONCLUSION

In the present paper we analyzed mass and heat transport in reactors for epitaxy from gas phase. Based on the analysis we obtain, that increasing of frequency of rotation of substrate and inlet speed of mixture of gases leads to increasing homogeneity of properties of epitaxial layer. Power of heating of reaction zone depends on speed of mixture of gas-reagents and area of reaction zone. Concentration of mixture of gases-reagents weakly depends on diffusion coefficient and viscosity in working area of parameters. In this paper we also introduce an analytical approach to model mass and heat transport in reactors for epitaxy from gas phase.

ACKNOWLEDGMENTS

This work is supported by the agreement of August 27, 2013 No 02 B 49.21.0003 between The Ministry of education and science of the Russian Federation and Lobachevsky State University of Nizhni Novgorod and educational fellowship for scientific research of Government of Russian and of Nizhny Novgorod State University of Architecture and Civil Engineering.

REFERENCES

- [1] I.P.Stepanenko; Basis of microelectronics. Moscow, Soviet radio (in Russian), (1980).
- [2] V.G.Gusev, Yu.M.Gusev; Electronics Moscow, Higher School (in Russian), (1991).
- [3] V.I.Lachin, N.S.Savelov; Electronics Rostov-on-Don, Phenics, (2001).
- [4] A.AVorob'ev, V.VKorabl'ev, S.Yu.Karpov Semiconductors, **37(7)**, 98 (2003).
- [5] L.M.Sorokin, N.V.Veselov, M.P.Shcheglov, A.E.Kalmykov, A.A.Sitnikova, N.A.Feoktistov, A.V.Osipov, S.A.Kukushkin Technical Physics Letters, **34(22)**, 68 (2008).
- [6] V.V.Lundin, A.V.Sakharov, E.E.Zavarin, M.A.Sinitsin, A.E.Nikolaevâ, G.A.Mikhailovsky, P.N.Brunkov, V.V.Goncharov, B.YaBer, D.Yu Kazantsev, A.F.Tsatsul; Nikov Semiconductors, **43(7)**, 996 (2009).
- [7] Y.Li, L.E.Antonuk, Y.El-Mohri, Q.Zhao, H.Du, A.Sawant, Yi Wang; J.Appl.Phys, **99(6)**, 064501 (2006).
- [8] A.Chakraborty, H.Xing, M.D.Craven, S.Keller, T.Mates, J.S.Speck, S.P.Den Baars, U.K.Mishra; J.Appl.Phys., **96(8)**, 4494 (2004).
- [9] M.Mitsuhara, M.Ogasawara, H.Sugiura; J.Cryst.Growth, **183**, 38 (1998).
- [10] R.A.Talalaev, E.V.Yakovleva, S.Yu Karpova, Yu.N.Makarov; J.Cryst.Growth, **230**, 232 (2001).
- [11] A.V.Kovalenko, A.Yu.Mekekechko; Semiconductors, **29(8)**, 1461 (1995).
- [12] B.Mitrovica, A.Gurarya, L.Kadinski, J.Cryst. Growth, **287**, 656 (2006).
- [13] R.Zuoa, H.Zhanga, X.-Lin Liu; J.Cryst.Growth, **293**, 498 (2006).
- [14] P.Zhang, H.Wei, G.Cong, W.Hu, H.Fan, J.JWu, Q.Zhu, X.Liu; Thin Solid Films, **516**, 925 (2008).
- [15] H.S.Carslaw, J.C.Jaeger; Conduction of heat in solids- Oxford: At the Clarendon Press, 1964488.
- [16] Yu.D.Sokolov; Applied Mechanics, **1(1)**, 23-35 (1955).
- [17] E.L.Pankratov, J.Comp.Theor.Nanoscience, **9(1)**, 41-49 (2012).
- [18] E.L.Pankratov, E.A.Bulaeva; J.Comp.Theor. Nanoscience, **10(4)**, 888-893 (2013).
- [19] E.L.Pankratov, E.A.Bulaeva; International Journal of Micro-Nano Scale Transport, **3(3)**, 119-130 (2012).
- [20] E.L.Pankratov, E.A.Bulaeva; Universal Journal of Materials Science, **1(4)**, 180-200 (2013).
- [21] E.L.Pankratov, E.A.Bulaeva; Reviews in Theoretical Science, **1(1)**, 58-82 (2013).
- [22] E.L.Pankratov, E.A.Bulaeva; Universal Journal of Materials Science, **1(4)**, 180-200 (2013).
- [23] E.L.Pankratov, E.A.Bulaeva; Reviews in Theoretical Science, **1(3)**, 305-316 (2013).
- [24] G.Korn, T.Korn; Mathematical Handbook for scientists and engineers, Definitions, Theorems and formulas for reference and review, 2nd Edition, McGraw-Hill Book Company, New York, (1968).