



Materials Science

An Indian Journal

Full Paper

MSAIJ, 14(6), 2016 [191-201]

On optimization of regimes of epitaxy from gas phase in a horizontal reactor

E.L.Pankratov^{1,3*}, 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)

³Nizhny Novgorod Academy of the Ministry of Internal Affairs of Russia, 3 Ankudinovskoe Shosse, Nizhny Novgorod, 603950, (RUSSIA)
E-mail: elp2004@mail.ru

ABSTRACT

In this paper we analyzed mass and heat transport in a horizontal 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. © 2016 Trade Science Inc. - INDIA

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. Several recommendations have been formulated 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. However 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]. However analytical approaches attracted an interest due to their visibility.

In this paper we analyzed mass and heat transport in a horizontal reactor from gas phase during growth an epitaxial layer. As a future development of works^[15-18] we obtain several conditions to improve properties of the epitaxial layer. Structure of reactor with induction heating is shown on Figure 1. We compare recently obtained in^[15-18] results for vertical reactor with new results for horizontal reactor.

Full Paper

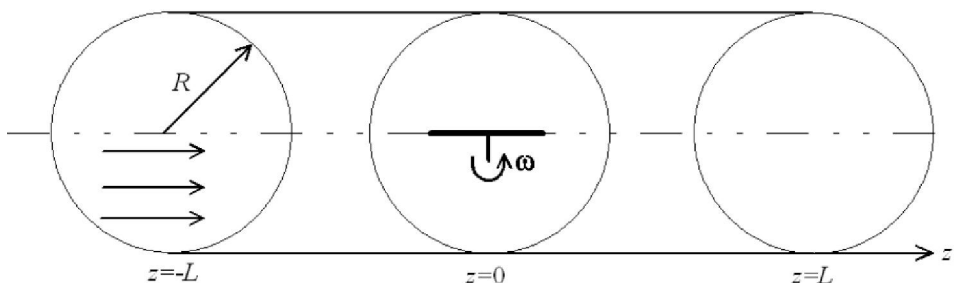


Figure 1a : A horizontal reactor for the gas phase epitaxy in neighborhoods of reaction zone $z \in [-L, L]$. Here z is the coordinate along reactor axis, R is the radius of reactor, ω is the frequency of rotation of keeper of substrate

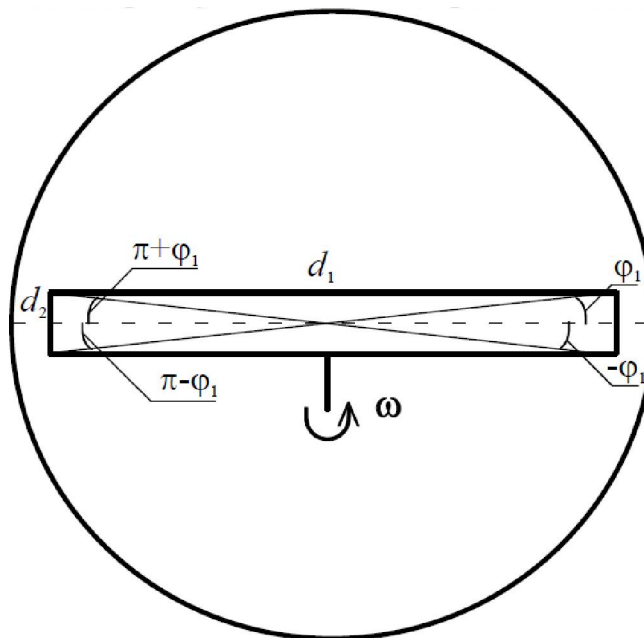


Figure 1b : View from side on keeper of substrate and approximation of the keeper by oblique lines with angle ϕ_1

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]

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

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

$$\begin{aligned} C(\mathbf{r}, \varphi, -L, t) = C_0, \quad C(\mathbf{r}, -\varphi_1, z, t) = C(\mathbf{r}, \varphi_1, z, t) = C(\mathbf{r}, \pi - \varphi_1, z, t) = C(\mathbf{r}, \pi + \varphi_1, z, t), \quad C(\mathbf{r}, \varphi, z, 0) = \\ = C_0 \delta(z+L), \quad C(0, \varphi, z, t) \neq \infty, \quad C(r, \varphi, z, t)|_S = 0, \quad T(\mathbf{r}, -\varphi_1, z, t) = T(\mathbf{r}, \varphi_1, z, t) = T(\mathbf{r}, \pi - \varphi_1, z, t) = \\ = T(\mathbf{r}, \pi + \varphi_1, z, t), \quad T(\mathbf{r}, \varphi, z, 0) = T_r, \quad T(0, \varphi, z, t) \neq \infty, \quad v_z(\mathbf{r}, \varphi, 0, t) = 0, \quad v_z(\mathbf{r}, \varphi, L, 0) = V_0, \quad v_\varphi(\mathbf{r}, \varphi, z, 0) = 0, \\ -\lambda \frac{\partial T(r, \varphi, z, t)}{\partial r} \Big|_S = \sigma T^4(R, \varphi, z, t), \quad \frac{\partial T(r, \varphi, z, t)}{\partial \varphi} \Big|_{\varphi=0} = \frac{\partial T(r, \varphi, z, t)}{\partial \varphi} \Big|_{\varphi=2\pi}, \end{aligned} \quad (4)$$

$$\frac{\partial C(r, \varphi, z, t)}{\partial r} \Big|_{r=R} = 0, \quad \frac{\partial v_r(r, \varphi, z, t)}{\partial r} \Big|_{r=0} = 0,$$

$$\frac{\partial v_r(r, \varphi, z, t)}{\partial r} \Big|_{r=R} = 0, \quad v_r(\mathbf{r}, -\varphi_1, z, t) = v_r(\mathbf{r}, \varphi_1, z, t) = v_r(\mathbf{r}, \pi - \varphi_1, z, t) = v_r(\mathbf{r}, \pi + \varphi_1, z, t), \quad v_\varphi(\mathbf{r}, -\varphi_1,$$

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

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

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

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

Full Paper

$$-v_r \frac{\partial v_r}{\partial r} - \frac{v_\varphi}{r} \frac{\partial v_\varphi}{\partial \varphi} - v_z \frac{\partial v_z}{\partial z} - \frac{1}{r} \frac{\partial}{\partial \varphi} \left(\frac{P}{\rho} \right) \quad (5b)$$

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

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

We determine solution of this system of equations by using of method of averaging of function corrections^[16-21]. 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

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

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

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

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

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

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

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

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

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

$$v_{2z} = V_0 + v \int_0^t \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial v_{1z}}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_{1z}}{\partial \varphi^2} + \frac{\partial^2 v_{1z}}{\partial z^2} \right] d\tau - \frac{\partial}{\partial z} \left(\int_0^t \frac{P}{\rho} d\tau \right) - \int_0^t (\alpha_{2r} + v_{1r}) \frac{\partial v_{1z}}{\partial r} d\tau - \int_0^t \frac{(\alpha_{2\varphi} + v_{1\varphi})}{r} \frac{\partial v_{1z}}{\partial \varphi} d\tau - \int_0^t (\alpha_{2z} + v_{1z}) \frac{\partial v_{1z}}{\partial z} d\tau. \quad (8f)$$

Farther we determine average values α_{2r} , $\alpha_{2\varphi}$, α_{2z} . The average values have been calculated by the following relations^[16-21]

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

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

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

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

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

Full Paper

$$\begin{aligned}
 & -t) dt - \frac{\pi}{8} \Theta^2 R^2 V_0^2 - \int_0^\Theta (\Theta - t) \int_0^R r \int_{-L}^{2\pi L} v_{1r} \frac{\partial v_{1r}}{\partial r} dz d\varphi dr dt - \int_0^\Theta \int_0^R \int_{-L}^{2\pi 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 r \int_{-L}^{2\pi L} \frac{\partial v_{1r}}{\partial r} dz d\varphi dr dt, B_2 = 1 + \int_0^\Theta \int_0^R \int_{-L}^{2\pi 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 r \int_{-L}^{2\pi 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 r \int_{-L}^{2\pi L} v_{1r} \frac{\partial v_{1r}}{\partial r} dz d\varphi dr dt - \int_0^\Theta (\Theta - t) \int_0^R r \int_{-L}^{2\pi 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 r \int_{-L}^{2\pi L} \frac{\partial v_{1z}}{\partial r} dz d\varphi dr dt, B_3 = \int_0^\Theta (\Theta - t) \int_0^R r \int_{-L}^{2\pi L} \frac{\partial v_{1z}}{\partial \varphi} dz d\varphi dr dt, \\
 & D_3 = v \int_0^\Theta (\Theta - t) \int_0^R r \int_{-L}^{2\pi 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 r \int_{-L}^{2\pi L} v_{1r} \frac{\partial v_{1z}}{\partial r} dz d\varphi dr dt - \int_0^\Theta (\Theta - t) \int_0^R r \int_{-L}^{2\pi 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^[22] and could be written as

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

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

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

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

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

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

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_{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-reagents

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

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

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

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

Substitution of the first-order approximations of temperature and concentration of gas mixer into relations (16) gives us the following results^[22]

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

Full Paper

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

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

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

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

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

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

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

$$\begin{aligned} \alpha_{2T} = & \left(\frac{\lambda \sigma}{c \pi \Theta R L} \int_0^\Theta (\Theta - t) \int_0^{2\pi} \int_{-L}^L T^4(R, \varphi, z, t) dz d\varphi dt - \int_0^\Theta (\Theta - t) \int_0^{2\pi} \int_{-L}^L T_1(R, \varphi, z, t) dz d\varphi dt \times \right. \\ & \times \frac{\lambda}{c \pi \Theta R^2 L} + \frac{\lambda}{c \pi \Theta R^2 L} \int_0^\Theta (\Theta - t) \int_0^{2\pi} \int_{-L}^L T_1(0, \varphi, z, t) dz d\varphi dt - \int_0^\Theta (\Theta - t) \int_0^{2\pi} \int_{-L}^L v_r(R, \varphi, z, t) \times \\ & \times \{ [\alpha_{2C} + C_1(R, \varphi, z, t)] T_1(R, \varphi, z, t) - \alpha_{1T} \alpha_{1C} \} dz d\varphi dt \frac{1}{\pi \Theta R L} - \frac{1}{\pi \Theta R^2 L} \int_0^\Theta (\Theta - t) \times \end{aligned}$$

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

DISCUSSION

In the present paper we analyzed dynamics of mass and heat transport during growth films from gas phase in a horizontal reactor 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 keeper of substrate ω (curve 2) in comparison with analogous curve for vertical reactor (curve 1). The Figure 3 shows, that dependence of concentration of material of epitaxial layer on diffusion coefficient D for vertical and horizontal reactors (curves 1 and 2, respectively). The figure shows monotonous decreasing of the

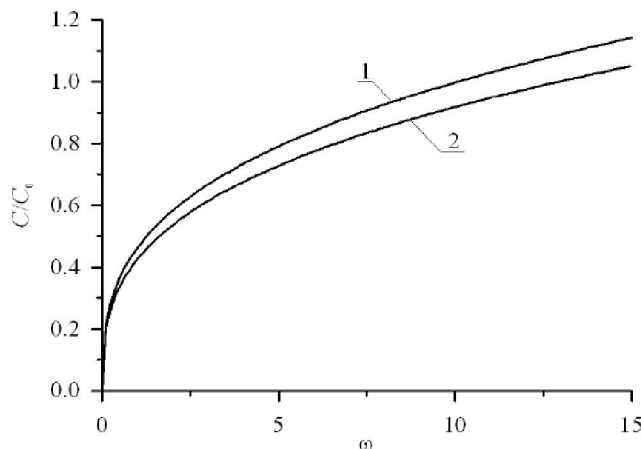


Figure 2 : Dependence of concentration of mixture of gases on frequency of rotation of substrate ω

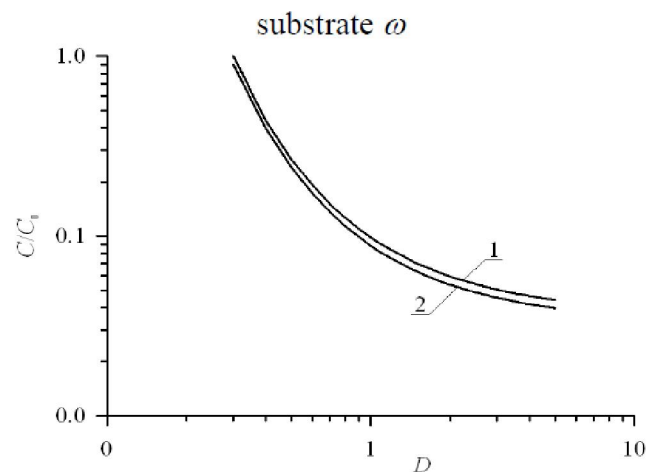


Figure 3 : Dependence of concentration of mixture of gases on diffusion coefficient D

Full Paper

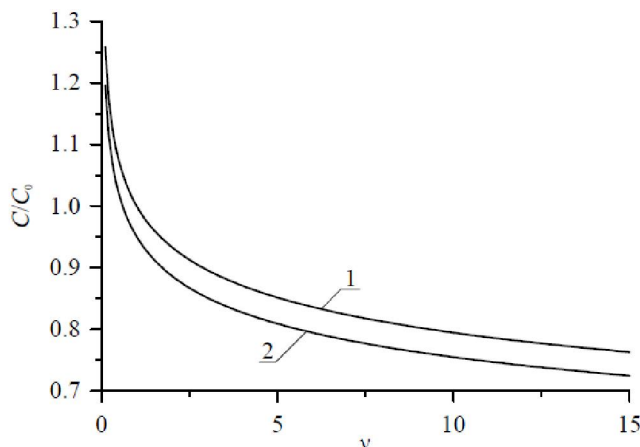


Figure 4 : Dependence of concentration of mixture of gases on kinematical viscosity ν

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 for vertical and horizontal reactors (curves 1 and 2, respectively). 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. Increasing of speed V_0 leads to increasing of concentration of reagents in reaction zone and to increasing of speed of growth of films.

It is known, that surface of manufacturing of an epitaxial layer in a horizontal reactor is inhomogenous (see, for example,^[23]). Increasing of temperature of growth leads to activation chemical reaction of gas-reagents and growth of films. At the same time one can find activation of diffusion of material of the manufacturing film. The acceleration leads to increasing homogeneity of surface of the film.

It is attracted an interest choosing of value of power of induction heating of growth area to compensate heat loss due to convective heat^[15]. In this

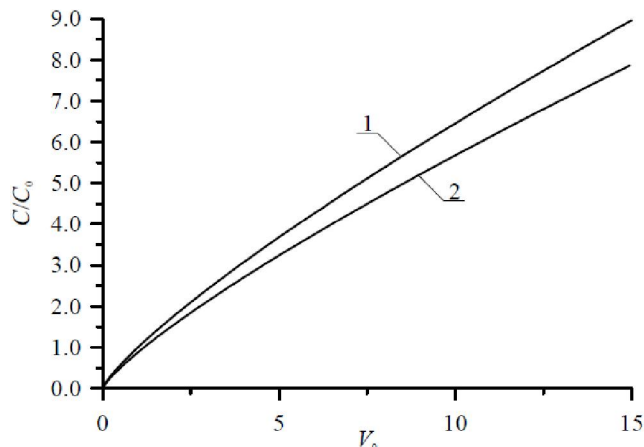


Figure 5 : Dependence of concentration of mixture of gases on inlet speed V_0

case time of heating of reactor zone ϑ could be estimated framework recently introduced approach^[24] 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:

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

It should be also noted, that all results, presented in Figures 2-5, have been calculated by using method of averaging of function corrections. Our several recent analytical results have been checked with numerical and experimental one.

CONCLUSION

In the present paper we analyzed mass and heat transport in a vertical reactor for epitaxy from gas phase. The result gives a possibility to formulate several recommendations to improve properties of epitaxial layers.

ACKNOWLEDGMENTS

This work is supported by the contract 11.G34.31.0066 of the Russian Federation Government, grant of Scientific School of Russia, 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 Univer-

sity 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.A.Vorob'ev, V.V.Korabl'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.Nikolaev, G.A.Mikhailovsky, P.N.Brunkov, V.V.Goncharov, B.Ya.Ber, 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 Den Baars, U.K.Mishra; J.Appl.Phys, **96(8)**, 4494 (2004).
- [9] M.Mitsuhashi, 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] E.L.Pankratov, E.A.Bulaeva; Universal Journal of Materials Science, **1(4)**, 180-200 (2013).
- [12] E.L.Pankratov, E.A.Bulaeva; International Journal of Computational Materials, **3(3)**, 1450013-1450026 (2014).
- [13] E.L.Pankratov, E.A.Bulaeva; Journal of Mechatronics, **2(2)**, 136-142 (2014).
- [14] E.L.Pankratov, E.A.Bulaeva; Reviews in Theoretical Science, **3(4)**, 365-398 (2015).
- [15] H.S.Carslaw, J.C.Jaeger; Conduction of heat in solids, - Oxford: At the Clarendon Press, 488 (1964).
- [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] 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).
- [23] V.G.Levich; Physicochemical hydrodynamics.Moscow: Science, (1962).
- [24] E.L.Pankratov, E.A.Bulaeva; Reviews in Theoretical Science, **1(3)**, 305-316 (2013).
- [25] E.L.Pankratov, E.A.Bulaeva; Universal Journal of Materials Science, **1(4)**, 180-200 (2013).