

On variation of Rate of Growth of Epitaxial Layers by Variation of Substrate Heating

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Abstract: In this paper, we estimate the rate of growth of epitaxial layers from the gas phase. We study dependence of the rate on the value of the heating of the sub-strate. By using the previously introduced approach of mass and heat transfer analysis, analytical dependencies of the considered rate on the parameters were obtained. In this paper based on recently introduced approach we analyzed mass and heat transport during growth of epitaxial layers in reactors for epitaxy from gas phase with sloping keeper with account native convection. Based on recently introduced approach we estimate rate of growth of films and analyzed depend-ences of the rate on physical and technological parameters.

Keywords: growth from gas phase, changing of growth rate, prognosis of technological process.

1 Introduction

At the present time different heterostructures are widely used to manufacture different devices of solid-state electronics. The most common methods for growing heterostructures are epitaxy from the gas and liquid phases, magnetron sputtering, molecular beam epitaxy. Manufacturing and using of heterostructures have been considered in large number of experimental works because of their wide using [1-11]. At the same time, a relatively small number of works are devoted to predicting the processes of epitaxy [12]. The main aim of the present paper is analysis the growth of epitaxial layers with changes in the values of parameters of the growth process taking into account natural convection.

In this paper we consider a reactor for epitaxy from the gas phase (see Fig. 1). This reactor consists of a casing, a substrate holder with a substrate, and a helix around the casing in the region of formation of the epitaxial layer in order to provide induction heating for activating the chemical reactions that occur during the decomposition of reagents and the formation of an epitaxial layer. A gaseous mixture of re-agents is supplied to the inlet of the reaction chamber together with the carrier gas. The main goal of this paper is to estimate the rate of growth of an epitaxial layer and to analyze its dependence on the substrate temperature.

2 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 [13]

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

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 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 solvi

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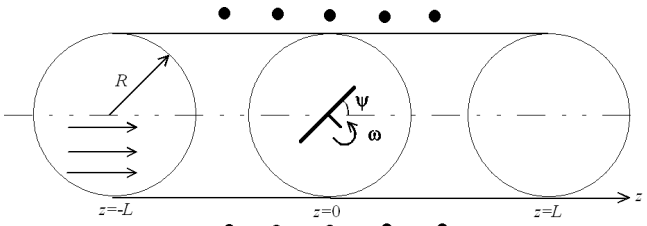


Fig. 1a: Structure of reactor for gas phase epitaxy with sloping keeper of substrate.

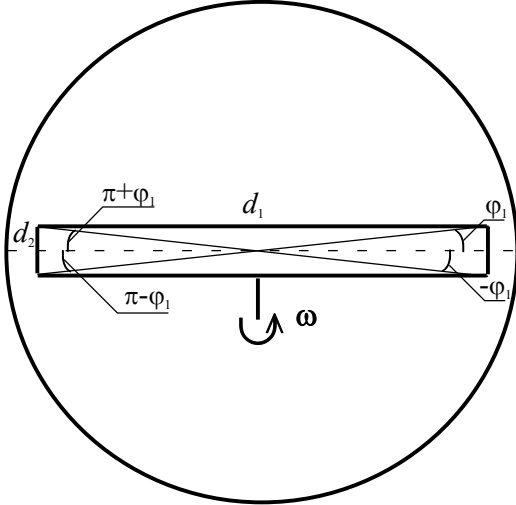


Fig. 1b: View from side of keeper of substrate and approximation of the keeper by sloping lines with angle of sloping φ_1 .

ing 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

$$\begin{aligned} C(r, \varphi, -L, t) &= C_0, C(r, -\varphi_1, z, t) = C(r, \varphi_1, z, t) = C(r, \pi - \varphi_1, z, t) = \\ &= C(r, \pi + \varphi_1, z, t), C(r, \varphi, z, 0) = C_0 \delta(z+L), C(0, \varphi, z, t) \neq \infty, \\ C(r, \varphi, z, t) \Big|_S &= 0, T(r, -\varphi_1, z, t) = T(r, \varphi_1, z, t) = T(r, \pi - \varphi_1, z, t) = \end{aligned}$$

$$= T(r, \pi + \varphi_1, z, t), \left. \frac{\partial C(r, \varphi, z, t)}{\partial r} \right|_{r=R} = 0, T(r, \varphi, z, 0) = T_r,$$

$$-\lambda \left. \frac{\partial T(r, \varphi, z, t)}{\partial r} \right|_S = \sigma T^4(R, \varphi, z, t), T(0, \varphi, z, t) \neq \infty,$$

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

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

$$v_r(r, -\varphi_1, z, t) = v_r(r, \varphi_1, z, t) = v_r(r, \pi - \varphi_1, z, t) = v_r(r, \pi + \varphi_1, z, t),$$

$$v_\varphi(r, -\varphi_1, z, t) = v_\varphi(r, \varphi_1, z, t) = v_\varphi(r, \pi - \varphi_1, z, t) = v_\varphi(r, \pi + \varphi_1, z, t),$$

$$v_z(r, -\varphi_1, z, t) = v_z(r, \varphi_1, z, t) = v_z(r, \pi - \varphi_1, z, t) = v_z(r, \pi + \varphi_1, z, t),$$

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

$$v_z(r \pm d_2/2, \varphi, z \in [-d_2/2, d_2/2], 0) = \omega z \cdot \cos \psi \operatorname{tg}(\varphi_1), \quad (4)$$

$$v_\varphi(r, \varphi, L, t) = 0, v_\varphi(0, \varphi, z, t) \neq \infty, v_z(r, \varphi, 0, t) = 0, v_z(r, \varphi, L, t) = V_0,$$

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

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

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

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

We determine solution of this system of equations by using of method of averaging of function corrections [14-19]. 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

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

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.

$$v_{1r} = -\frac{\partial}{\partial r} \int_0^t \frac{P}{\rho} d\tau, \quad v_{1\phi} = -\frac{1}{r} \frac{\partial}{\partial \phi} \int_0^t \frac{P}{\rho} d\tau,$$

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

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

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

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

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

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

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

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

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

Farther we determine average values α_{2r} , $\alpha_{2\phi}$, α_{2z} . The average values have been calculated by the following relations [14-19]

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

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

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

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

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

where $A_1 = 1 + \int_0^\Theta (\Theta - t) \int_0^R \int_0^{2\pi} \int_{-L}^L \frac{\partial v_{1r}}{\partial r} dz d\phi dr dt$, $B_1 = \int_0^\Theta (\Theta - t) \times \int_0^R \int_0^{2\pi} \int_{-L}^L \frac{\partial v_{1r}}{\partial \phi} dz d\phi dr dt$, $C_1 = C_2 = \frac{\pi}{2} \Theta^2 R^2 V_0$, $D_1 = v \times \int_0^\Theta (\Theta - t) \int_0^R \int_0^{2\pi} \int_{-L}^L \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial v_{1r}}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_{1r}}{\partial \phi^2} + \frac{\partial^2 v_{1r}}{\partial z^2} \right] dz d\phi dr dt - \frac{\pi}{8} \Theta^2 R^2 V_0^2 - \int_0^\Theta (\Theta - t) \int_0^R \int_0^{2\pi} \int_{-L}^L v_{1r} \frac{\partial v_{1r}}{\partial r} dz d\phi dr dt - \int_0^\Theta (\Theta - t) \times \int_0^R \int_0^{2\pi} \int_{-L}^L v_{1\phi} \frac{\partial v_{1r}}{\partial \phi} dz d\phi dr dt$, $A_2 = \int_0^\Theta (\Theta - t) \int_0^R \int_0^{2\pi} \int_{-L}^L \frac{\partial v_{1r}}{\partial r} dz d\phi dr \times (\Theta - t) dt$, $B_2 = 1 + \int_0^\Theta (\Theta - t) \int_0^R \int_0^{2\pi} \int_{-L}^L \frac{\partial v_{1r}}{\partial \phi} dz d\phi dr dt$, $D_2 = v \int_0^\Theta (\Theta - t) \int_0^R \int_0^{2\pi} \int_{-L}^L \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial v_{1\phi}}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_{1\phi}}{\partial \phi^2} + \frac{\partial^2 v_{1\phi}}{\partial z^2} \right] dz d\phi \times (\Theta - t) dr dt - \int_0^\Theta (\Theta - t) \int_0^R \int_0^{2\pi} \int_{-L}^L v_{1r} \frac{\partial v_{1r}}{\partial r} dz d\phi dr dt - \int_0^\Theta (\Theta - t) \times \int_0^R \int_0^{2\pi} \int_{-L}^L v_{1\phi} \frac{\partial v_{1r}}{\partial \phi} dz d\phi dr dt - \frac{\pi}{8} \Theta^2 R^2 V_0^2$, $C_3 = 1 + \frac{\pi}{2} \Theta^2 R^2 V_0$, $A_3 = \int_0^\Theta (\Theta - t) \int_0^R \int_0^{2\pi} \int_{-L}^L \frac{\partial v_{1z}}{\partial r} dz d\phi dr dt$, $B_3 = \int_0^\Theta (\Theta - t) \int_0^R \int_0^{2\pi} \int_{-L}^L \frac{\partial v_{1z}}{\partial \phi} dz d\phi dr dt$, $D_3 = v \int_0^\Theta (\Theta - t) \int_0^R \int_0^{2\pi} \int_{-L}^L \left[\frac{\partial^2 v_{1z}}{\partial z^2} + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial v_{1z}}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_{1z}}{\partial \phi^2} \right] dz d\phi dr dt - \frac{\pi}{8} \Theta^2 R^2 V_0^2 - \int_0^\Theta (\Theta - t) \int_0^R \int_0^{2\pi} \int_{-L}^L v_{1r} \frac{\partial v_{1z}}{\partial r} dz d\phi dr dt - \int_0^\Theta (\Theta - t) \int_0^R \int_0^{2\pi} \int_{-L}^L v_{1\phi} \frac{\partial v_{1z}}{\partial \phi} dz d\phi \times r dr (\Theta - t) dt$.

Solution of the above system of equations could be determined by standard approaches [20] and could be written as

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

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

In this section we obtained components of velocity of stream of mixture of materials in gas phase, which are used for growth of hetero structure, 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.

Now let us rewrite Eqs.(1) and (3) by using cylindrical system of coordinate

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

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

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

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

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

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

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

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

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

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

$$\begin{aligned} c \cdot T_2(r, \varphi, z, t) = \lambda \int_0^t \frac{\partial^2 T_1(r, \varphi, z, \tau)}{\partial r^2} d\tau + \lambda \frac{1}{r^2} \int_0^t \frac{\partial^2 T_1(r, \varphi, z, \tau)}{\partial \varphi^2} d\tau + \\ + \lambda \int_0^t \frac{\partial^2 T_1(r, \varphi, z, \tau)}{\partial z^2} d\tau + \int_0^t p(r, \varphi, z, \tau) d\tau - c \cdot \frac{\partial}{\partial r} \int_0^t \{v_r(r, \varphi, z, \tau) \cdot \\ \cdot [\alpha_{2C} + C_1(r, \varphi, z, \tau)] \cdot [\alpha_{2T} + T_1(r, \varphi, z, \tau)]\} d\tau + T_r - \\ - \frac{c}{r} \frac{\partial}{\partial \varphi} \int_0^t \{[\alpha_{2C} + C_1(r, \varphi, z, \tau)] \cdot [\alpha_{2T} + T_1(r, \varphi, z, \tau)] \cdot \\ \cdot v_\varphi(r, \varphi, z, \tau)\} d\tau - c \cdot \frac{\partial}{\partial z} \int_0^t \{v_z(r, \varphi, z, \tau) \cdot [\alpha_{2C} + C_1(r, \varphi, z, \tau)] \cdot \\ \cdot [\alpha_{2T} + T_1(r, \varphi, z, \tau)]\} d\tau, \end{aligned} \quad (16)$$

$$\begin{aligned}
 C_2(r, \varphi, z, t) = & \frac{1}{r} \frac{\partial}{\partial r} \int_0^t r D \frac{\partial C_1(r, \varphi, z, \tau)}{\partial r} d\tau + \frac{1}{r^2} \frac{\partial}{\partial \varphi} \int_0^t D \times \\
 & \times \frac{\partial C_1(r, \varphi, z, \tau)}{\partial \varphi} d\tau + \frac{\partial}{\partial z} \int_0^t D \times \frac{\partial C_1(r, \varphi, z, \tau)}{\partial z} d\tau - \\
 & - \frac{1}{r} \frac{\partial}{\partial r} \left\{ r \int_0^t [\alpha_{2C} + C_1(r, \varphi, z, \tau)] \cdot v_r(r, \varphi, z, \tau) d\tau \right\} - \\
 & - \frac{1}{r} \frac{\partial}{\partial \varphi} \int_0^t v_\varphi(r, \varphi, z, \tau) \cdot [\alpha_{2C} + C_1(r, \varphi, z, \tau)] d\tau + C_0 \delta(z+L) - \\
 & - \frac{\partial}{\partial z} \int_0^t [\alpha_{2C} + C_1(r, \varphi, z, \tau)] \cdot v_z(r, \varphi, z, \tau) d\tau. \quad (17)
 \end{aligned}$$

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

$$\begin{aligned}
 \alpha_{2T} = & \frac{1}{\pi \Theta R^2 L} \int_0^R \int_0^{2\pi} \int_{-L}^L (T_2 - T_1) dz d\varphi dr dt \\
 \alpha_{2C} = & \frac{1}{\pi \Theta R^2 L} \int_0^R \int_0^{2\pi} \int_{-L}^L (C_2 - C_1) dz d\varphi dr dt. \quad (18)
 \end{aligned}$$

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

$$\begin{aligned}
 \alpha_{2T} = & \left(\frac{\lambda \sigma}{c \pi \Theta R L} \int_0^\Theta (\Theta - t) \int_0^{2\pi} \int_{-L}^L T^4(R, \varphi, z, t) dz d\varphi dt - \right. \\
 & - \frac{\lambda}{c \pi \Theta R^2 L} \int_0^\Theta (\Theta - t) \int_0^{2\pi} \int_{-L}^L T_1(R, \varphi, z, t) dz d\varphi dt + \\
 & + \frac{\lambda}{c \pi \Theta R^2 L} \int_0^\Theta (\Theta - t) \int_0^{2\pi} \int_{-L}^L T_1(0, \varphi, z, t) dz d\varphi dt - \int_0^\Theta (\Theta - t) \times \\
 & \times \int_0^{2\pi} \int_{-L}^L \{ [\alpha_{2C} + C_1(R, \varphi, z, t)] T_1(R, \varphi, z, t) - \alpha_{1T} \alpha_{1C} \} \times \\
 & \times v_r(R, \varphi, z, t) dz d\varphi dt - \frac{1}{\pi \Theta R L} - \frac{1}{\pi \Theta R^2 L} \int_0^\Theta (\Theta - t) \times \\
 & \times \int_0^{R/2} \int_0^{2\pi} \int_{-L}^L \{ T_1(r, \varphi, z, t) [\alpha_{2C} + C_1(r, \varphi, z, t)] - \alpha_{1T} \alpha_{1C} \} \times \\
 & \times v_r(r, \varphi, z, \tau) dz d\varphi r dr dt - \frac{V_0}{\pi \Theta R^2 L} \int_0^\Theta (\Theta - t) \int_0^R r \times \\
 & \times \int_0^{2\pi} [(\alpha_{2C} + C_0) \cdot T_1(r, \varphi, L, t) - \alpha_{1T} \alpha_{1C}] d\varphi dr dt \left\{ 1 + \frac{1}{\pi \Theta R L} \times \right.
 \end{aligned}$$

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

3 Discussion

3.1 Main Relations to Estimate Rate of Growth

In this section, we will estimate the rate of growth of epitaxial layers. The required velocity is determined by the following relation [21]: $V_g \approx DC/\delta\rho$, where D is the diffusion coefficient of the gas mixture, C is the concentration of the gas mixture, δ is the thickness of the diffusion layer, and ρ is the density of the gas mixture. The thickness of the diffusion layer can be determined using the following relation [21]: $\delta \approx 1.6\sqrt[3]{D\nu} \sqrt{\nu/\omega}$, where ν is the viscosity of the gas mixture, ω is the rotation frequency of the substrate holder.

3.2 Main Results

The Fig. 2 shows the dependence of the considered growth rate on the frequency of rotation of the substrate. Curve 1 describes the dependence of the growth rate on the frequency of rotation of the substrate at atmospheric pressure without taking natural convection into account (at a low growth temperature, the value of natural convection can be neglected). Curve 2 describes the dependence of the speed of growth on the frequency of rotation of the substrate at a pressure that is reduced by an order of magnitude without taking natural convection into account. Curve 3 describes the dependence of the speed of growth on the frequency of rotation of the substrate at atmospheric pressure, taking into account natural convection. It follows from this figure that an increase in the frequency of rotation of the substrate holder leads to a more uniform growth of the material deposited on the substrate along its radius. The increasing in

the growth temperature leads to an increasing in the contribution of natural convection and the slowing down of the growth of epitaxial layers. The Fig. 3 shows the dependence of the growth speed of the epitaxial layer on the diffusion coefficient D . Curve 1 describes the dependence of the growth rate on the diffusion coefficient at atmospheric pressure without taking natural convection into account. Curve 2 describes the dependence of the growth rate on the diffusion coefficient at atmospheric pressure with decreased value pressure on one order than natural convection. Curve 3 describes the dependence of the growth rate on the diffusion coefficient at atmospheric pressure at atmospheric pressure with allowance for natural convection. From this figure we see a monotonous increase in the considered velocity. An increase in the value of the diffusion coefficient leads to an increase in the rate of transfer of the gas mixture, which leads to an increase in the rate of growth of the epitaxial layer. The value of the diffusion coefficient can be reduced by decreasing the growth temperature. However, as the growth temperature decreases, the chemical reaction slows down. The dependence of the growth rate of the epitaxial layer on the kinematic viscosity ν is shown in Fig. 4. The designations of the curves in this figure are the same as in the previous two. The decrease in the growth rate with increasing viscosity is due to the slowing down of the transfer of the gas mixture. Dependences of the growth speed of the epitaxial layer on the speed of the gas mixture at the inlet to the reaction zone V_0 is shown in Fig. 5. Curve 1 describes the dependence of the growth speed on the velocity of the mixture of gases at the inlet to the reaction zone at atmospheric pressure without taking natural convection into account. Curve 2 describes the dependence of the growth speed on the speed of the gas mixture at the entrance to the reaction zone at decreased value of pressure on one order, without taking natural convection into account. Curve 3 describes the dependence of the growth speed on the speed of the gas mixture at the inlet to the reaction zone at atmospheric pressure, taking natural convection into account. An increase in the V_0 speed leads to an increase in the concentration of the gas mixture in the reaction zone and, as a consequence, to an acceleration of the growth of the epitaxial layer. It also follows from the analysis that a decrease in the pressure in the reactor makes it possible to reduce the inertia of the processes occurring in it. Natural convection leads to a slowing down of the growth of the epitaxial layer.

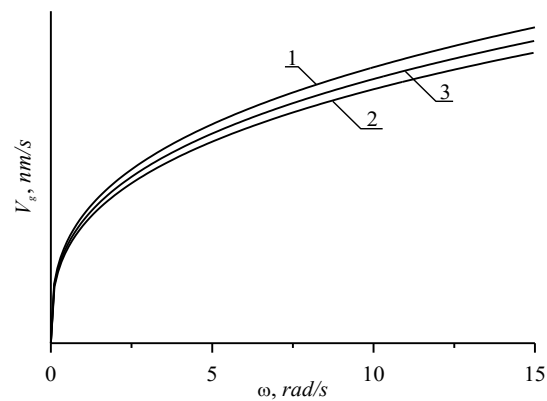


Fig. 2a: Dependence of growth speed on frequency of rotation of substrate ω . Curve 1 corresponds to vertical reactor. Curve 2 corresponds to horizontal reactor. Curve 3 corresponds to average value of sloping angle (i.e. $\psi = 45^\circ$) of keeper of substrate in comparison with direction of flow gazes.

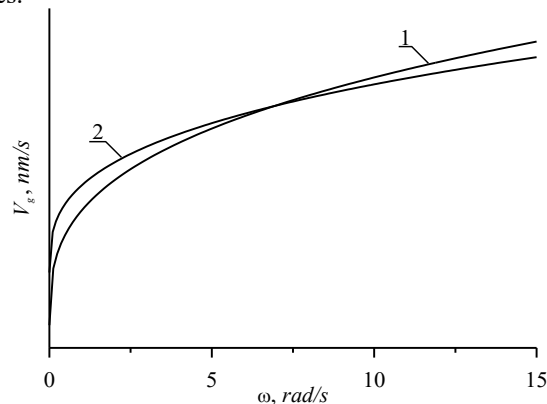


Fig. 2b: Dependence of growth speed on frequency of rotation of substrate ω . Curve 1 corresponds to atmospheric pressure. Curve 2 corresponds to smaller pressure.

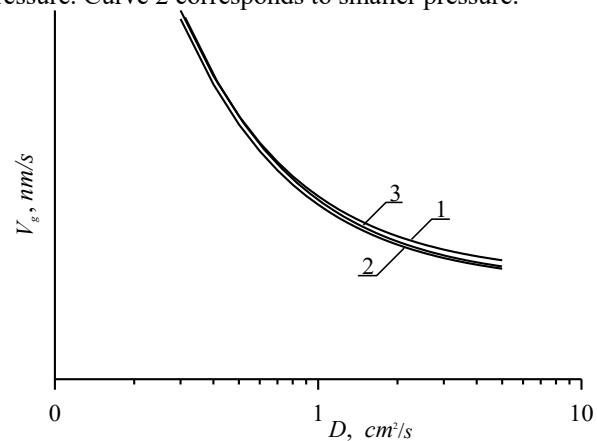


Fig. 3a: Dependence of growth speed on diffusion coefficient D . Curve 1 corresponds to vertical reactor. Curve 2 corresponds to horizontal reactor. Curve 3 corresponds to average value of sloping angle (i.e. $\psi = 45^\circ$) of keeper of substrate in comparison with direction of flow gazes.

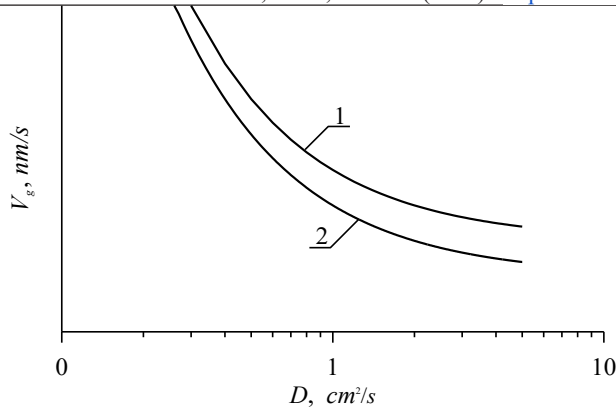


Fig. 3b: Dependence of growth speed on diffusion coefficient D . Curve 1 corresponds to atmospheric pressure. Curve 2 corresponds to smaller pressure.

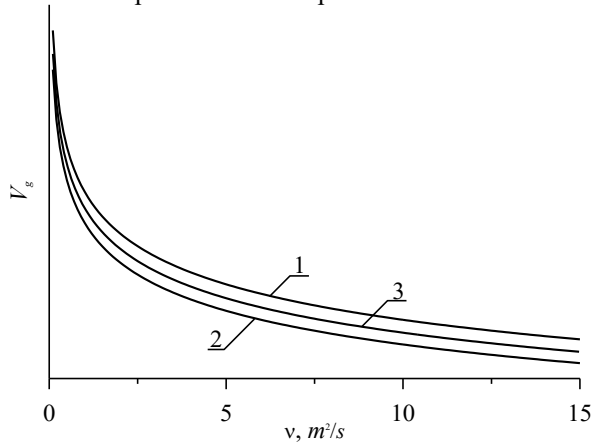


Fig. 4a: Dependence of growth speed on viscosity ν . Curve 1 corresponds to vertical reactor. Curve 2 corresponds to horizontal reactor. Curve 3 corresponds to average value of sloping angle (i.e. $\psi=45^\circ$) of keeper of substrate in comparison with direction of flow gazes.

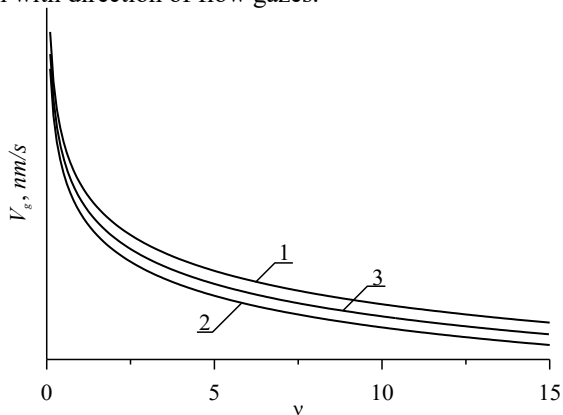


Fig. 4b: Dependence of growth speed of gases on viscosity ν . Curve 1 corresponds to atmospheric pressure. Curve 2 corresponds to smaller pressure.

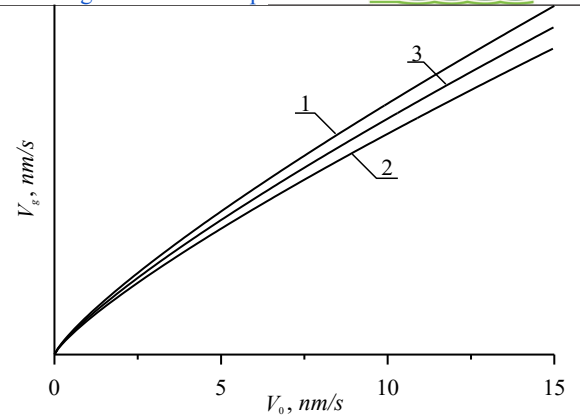


Fig. 5a: Dependence of growth speed on inlet velocity V_0 . Curve 1 corresponds to vertical reactor. Curve 2 corresponds to horizontal reactor. Curve 3 corresponds to average value of sloping angle (i.e. $\psi=45^\circ$) of keeper of substrate in comparison with direction of flow gazes.

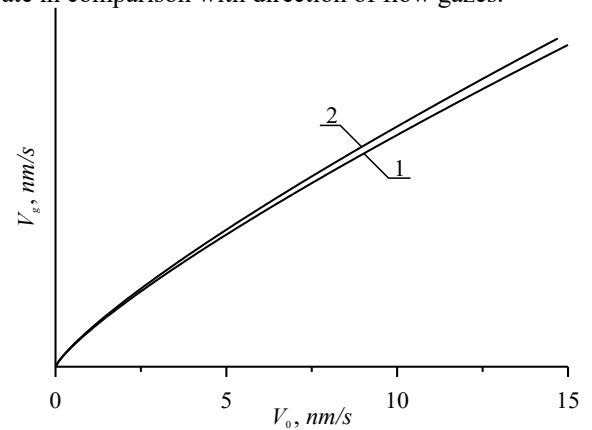


Fig. 5b: Dependence of growth speed on inlet velocity V_0 . Curve 1 corresponds to atmospheric pressure. Curve 2 corresponds to smaller pressure.

4 Conclusions

In this paper, we estimate the rate of growth of epitaxial layers from the gas phase. We study its dependence on the amount of heating of the substrate. By using the previously proposed mass and heat transfer analysis, analytical dependencies of the considered velocity on the parameters were obtained.

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