International Journal of Advances in Electrical Engineering

E-ISSN: 2708-4485
P-ISSN: 2708-4477
IJEDN 2022; 3(2): 88-104

www.electronicnetjournal.com
Received: 13-05-2022
Accepted: 15-06-2022

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Influence of substrate preliminary processing on the properties of the heterostructure

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Abstract
In this paper we analyze effect of preliminary processing of substrate on properties of the grown heterostructure. It has been shown that growth of an epitaxial layer on a buffer layer after preliminary (before starting of growth) annealing makes it possible to decrease of value of miss match-induced stress. An analytical approach has been introduced for analysis of mass and heat transfer in a multilayer structures with account miss match-induced stress.

Keywords: Gas phase epitaxy, improvement of properties of films, analytical approach for modeling

Introduction

To manufacture of various devices of solid-state electronics, heterostructures of different configurations are frequently used. For their growth different methods could be used: gas-phase and liquid-phase epitaxy, sputtering of materials in magnetrons and molecular beam epitaxy. The manufacturing and using of heterostructures in different devices was described in a large number of experimental works [1-11]. At the same time, fewer works are describing prediction of epitaxy processes [12, 13]. In this paper we consider a vertical reactor for gas phase epitaxy (see Fig. 1). The reactor consists of an external casing, a substrate holder with a substrate, and a spiral around the casing in area of the substrate to generate induction heating to activate chemical reactions of decay of reagents and to growth of the epitaxial layer. A gaseous mixture of reagents together with a gas-carrier inputs into inlet of the reaction chamber. At the first stage of the growth of the heterostructure a buffer layer was grown on a substrate. Next the resulting structure was annealed. After that an epitaxial layer was grown. The main aim of this paper was analyzed of changing of the properties of the heterostructure with account of the considered annealing. An accompanying aim of this paper is introduction of an analytical approach for analysis of mass and heat transfer in multilayer structures with account their nonlinearity, changes of parameters of processes in space and time, miss match-induced stresses.

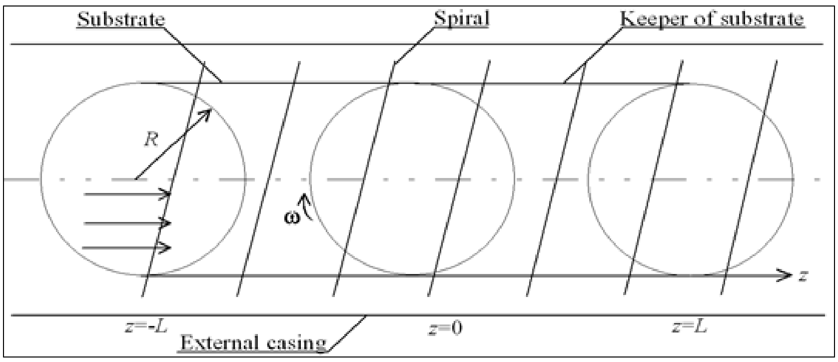

Fig 1: A reactor for the gas phase epitaxy in neighborhoods of reaction zone

Method of solution

The aim of the present paper will be solved by analyzing the spatio-temporal distribution of distribution of temperature and the concentration of the deposited material. The required temperature distribution was calculated by solving of the following boundary value problem [14].

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

where vector $\vec{v}$ is the speed of flow of the considered mixture of gases; parameter c is the capacity of heat; function T (r, φ, z, t) is the distribution of temperature in space and time; function p (r, φ, z, t) describes the power density, which standing out in the considered system substrate - keeper; r, φ and z are the cylindrical coordinates; t is the current time; function C (r, φ, z, t) describes the distribution of concentration of mixture of gases in space and time; parameter λ describes the conductivity of heat. 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 modulus of mean squared speed of the gas molecules, which equal to $\bar{v}=\sqrt{2kT/m}$, $\bar{l}$ is the average free path of gas molecules between collisions, c_v is the heat capacity at constant volume, ρ is the density of gas.
To solve this boundary problem one shall to take into account moving of mixture of gases and concentration of this mixture. We calculate the required values by solving the equation of Navier-Stokes and the second Fourier law. We also assume that radius of keeper of substrate R essentially larger, than thickness of diffusion and near-boundary layers. We also assume, that stream of gas is laminar. In this situation the appropriate equations could be written as

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

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

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

C (r, φ, -L, t) = C_0, C (r, φ, 0, t) = 0, C (r, 0, z, t) = C (r, 2π, z, t), C (r, φ, z, 0) = $C_0\delta(z + L)$,

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

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

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

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

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

T (0, φ, z, t) $\neq\infty$, v_r (r, φ, -L, t) = 0,
v_r (r, φ, 0, t) = 0, v_r(r, φ, L, t) = 0, v_r(r, 0, z, t) = v_r(r, 2π, z, t), v_r (0, φ, z, t) $\neq\infty$, v_φ (r, φ, 0, t) = ωr,
v_φ (r, φ, -L, t) = 0, v_φ (r, φ, L, t) = 0, v_φ(r, 0, z, t) = v_φ(r, 2π, z, t), v_φ(0, φ, z, t) $\neq\infty$, v_z(r, φ, -L, t) = V_0,

$v_z(r,\varphi,0,t)=\bar{v}_z$, $v_z(r, \varphi, L, t) = 0$, $v_z(r, 0, z, t) = v_z(r, 2\pi, z, t)$, $v_z(0, \varphi, z, t) \neq \infty$, $v_r(r, \varphi, z, 0) = 0$, $v_\varphi(r, \varphi, z, 0) = 0$, $v_z(r, \varphi, -L, 0) = V_0$.

Here parameter σ is equal to σ=5, 67·10^{-8} $W \cdot m^{-2} \cdot K^{-4}$, parameter T_r describes the room temperature, parameter ω describes the frequency of rotation of substrate.

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

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

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

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

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

We determine solution of this system of equations by using of method of averaging of function corrections [15-20]. Framework this approach to determine the first-order approximation of components of speed of flow of mixture of gases we replace of the required functions on their average values $v_r \to a_{1r}$, $v_\varphi \to a_{1\varphi}$, $v_z \to a_{1z}$ in right sides of equations of system (5). After the replacement we obtain equations for the first-order approximations of the components

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

Solutions of the above equations could be written as

$$v_{1r}=-\frac{\partial}{\partial r}\int_0^t\frac{P}{\xi}d\tau,\ v_{1\varphi}=-\frac{1}{r}\frac{\partial}{\partial \varphi}\int_0^t\frac{P}{\xi}d\tau,\ v_{1z}=-\frac{\partial}{\partial z}\int_0^t\frac{P}{\xi}d\tau. \tag{7}$$

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

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

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

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

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

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

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

Integration of the above equations leads to the following result

$$v_{2r}=\nu\int_0^t\left(\frac{\partial^2 v_{1r}}{\partial r^2}+\frac{\partial^2 v_{1r}}{\partial r\,\partial z}-\frac{\partial^2 v_{1r}}{\partial z^2}+\frac{\partial^2 v_{1z}}{\partial r\,\partial z}\right)d\tau-\frac{\partial}{\partial r}\left(\int_0^t\frac{P}{\xi}d\tau\right)-$$

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

$$v_{2\varphi}=\nu\int_0^t\left(\frac{1}{r}\frac{\partial^2 v_{1r}}{\partial r\,\partial \varphi}+\frac{2}{r^2}\frac{\partial^2 v_{1\varphi}}{\partial \varphi^2}-\frac{1}{r^2}\frac{\partial^2 v_{1r}}{\partial \varphi\,\partial z}+\frac{\partial^2 v_{1\varphi}}{\partial z^2}\right)d\tau-\frac{1}{r}\frac{\partial}{\partial \varphi}\left(\int_0^t\frac{P}{\xi}d\tau\right)-$$

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

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

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

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

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

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

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

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

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

Where $A_1 = 1 + \int_0^{\Theta} (\Theta - t) \int_0^R r \int_0^{2\pi} \int_{-L}^{L} \frac{\partial v_{1r}}{\partial r} d\,z\,d\,\varphi\,d\,r\,d\,t$, $B_1 = \int_0^{\Theta} (\Theta - t) \int_0^R \int_0^{2\pi} \int_{-L}^{L} \frac{\partial v_{1r}}{\partial \varphi} d\,z\,d\,\varphi\,d\,r\,d\,t$

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

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

$\times (\Theta - t)\,d\,t$, $A_2 = \int_0^{\Theta} (\Theta - t) \int_0^R r \int_0^{2\pi} \int_{-L}^{L} \frac{\partial v_{1r}}{\partial r} d\,z\,d\,\varphi\,d\,r\,d\,t$, $B_2 = 1 + \int_0^{\Theta} \int_0^R \int_0^{2\pi} \int_{-L}^{L} \frac{\partial v_{1r}}{\partial \varphi} d\,z\,d\,\varphi\,d\,r\,(\Theta -$

$- t)\,d\,t$, $D_2 = \nu \int_0^{\Theta} (\Theta - t) \int_0^R r \int_0^{2\pi} \int_{-L}^{L} \left(\frac{1}{r} \frac{\partial^2 v_{1r}}{\partial r \partial \varphi} + \frac{2}{r^2} \frac{\partial^2 v_{1\varphi}}{\partial \varphi^2} - \frac{1}{r^2} \frac{\partial^2 v_{1r}}{\partial \varphi \partial z} + \frac{\partial^2 v_{1\varphi}}{\partial z^2} \right) d\,z\,d\,\varphi\,d\,r\,d\,t -$

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

$A_3 = \int_0^{\Theta} (\Theta - t) \int_0^R r \int_0^{2\pi} \int_{-L}^{L} \frac{\partial v_{1z}}{\partial r} d\,z\,d\,\varphi\,d\,r\,d\,t$, $B_3 = \int_0^{\Theta} (\Theta - t) \int_0^R r \int_0^{2\pi} \int_{-L}^{L} \frac{\partial v_{1z}}{\partial \varphi} d\,z\,d\,\varphi\,d\,r\,d\,t$, $C_3 = 1 +$

$+ \frac{\pi}{2} \Theta^2 R^2 V_0$, $D_3 = \nu \int_0^{\Theta} (\Theta - t) \int_0^R r \int_0^{2\pi} \int_{-L}^{L} \left(\frac{\partial^2 v_{1r}}{\partial z^2} + \frac{\partial^2 v_{1z}}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2 v_{1z}}{\partial \varphi^2} \right) d\,z\,d\,\varphi\,d\,r\,d\,t - \int_0^{\Theta} (\Theta - t) \times$

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

Solution of the above system of equations could be determined by standard approaches [21] and could be written as

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

Where

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

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

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

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

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

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

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

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

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

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

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

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

We calculate distribution of temperature in space and time and the same distribution of concentration of mixture of gases we used the 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 a_{1T} and a_{1C} in right sides of the above equations. Farther we used recently consider algorithm to obtain the first-order approximations of temperature and concentration of gas mixture

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

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

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

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

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

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

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

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

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

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

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

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

$$\left.\left. + 1 + \Theta V_0 / R L \right\}^{-1} \right).$$

The second-order approximations of temperature and concentration of mixture of gases we determine framework the method of averaging of function corrections [15-20], i.e. by replacement of the required functions in right sides of equations (12) and (13) on the following sums $T \to a_{2T} + T_1$, $C \to a_{2C} + C_1$. In this case the second-order approximations of the above required functions could be written as

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

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

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

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

$$+ \int_0^t p(r,\varphi,z,\tau)\,d\,\tau + T_r, \qquad (16)$$

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

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

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

$$-\frac{\partial}{\partial z}\int_0^t [\alpha_{2C}+C_1(r,\varphi,z,\tau)]\cdot[v_z(r,\varphi,z,\tau)-\bar{v}_z(r,\varphi,z,\tau)]d\tau . \tag{17}$$

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

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

$$\alpha_{2C}=\frac{1}{\pi\Theta R^2 L}\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^{L}(C_2-C_1)\,d\,z\,d\,\varphi\,d\,r\,d\,t . \tag{18}$$

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

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

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

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

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

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

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

$$\times\int_0^\Theta(\Theta-t)\int_0^R r\int_0^{2\pi}\int_{-L}^{L}[v_r(r,\varphi,z,t)-\bar{v}_r(r,\varphi,z,t)]\cdot[\alpha_{2C}+C_1(r,\varphi,z,t)]\,d\,z\,d\,\varphi\,d\,r\,d\,t+(\alpha_{2C}+C_0)\times+2\Theta V_0/L\}^{-1}$$

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

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

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

After growing of the buffer layer we consider annealing the resulting two-layer structure. During the annealing one can find diffusion mixing of the heterostructure layers. Thermal diffusion in this case will be one-dimensional and perpendicular to the interface between the layers. But due to the mismatch of the lattice constants of these layers one can find miss match-induced stress. In this situation to describe the mixing of layers we use the second Fick's law in the following form [22, 23].

$$\frac{\partial \rho(x,y,z,t)}{\partial t}=\frac{\partial}{\partial z}\left[D\frac{\partial \rho(x,y,z,t)}{\partial z}\right]+\Omega\frac{\partial}{\partial x}\left[\frac{D_S}{kT}\nabla_S\mu(x,y,z,t)\int_0^{L_z}\rho(x,y,W,t)dW\right]+$$
$$+\Omega\frac{\partial}{\partial y}\left[\frac{D_S}{kT}\nabla_S\mu(x,y,z,t)\int_0^{L_z}\rho(x,y,W,t)dW\right] \qquad (19)$$

with initial and boundary conditions

$$\left.\frac{\partial \rho(x,y,z,t)}{\partial x}\right|_{x=0}=0,\ \left.\frac{\partial \rho(x,y,z,t)}{\partial x}\right|_{x=L_x}=0,\ \left.\frac{\partial \rho(x,y,z,t)}{\partial y}\right|_{y=0}=0,\ \left.\frac{\partial \rho(x,y,z,t)}{\partial y}\right|_{x=L_y}=0,$$
$$\left.\frac{\partial \rho(x,y,z,t)}{\partial z}\right|_{z=0}=0,\ \left.\frac{\partial \rho(x,y,z,t)}{\partial z}\right|_{x=L_z}=0,\ \rho(x,y,z,0)=f_\rho(x,y,z).$$

In the above relations the following denotations were introduced: Ω is the atomic volume of dopant; ∇_s is the symbol of surficial gradient; $\rho(x, y, z, T)$ is the diffusant concentration; $\int_0^{L_z}\rho(x,y,z,t)dz$ is the surficial concentration of the considered diffusant on interface between layers of heterostructure; $\mu(x, y, z, t)$ is the chemical potential due to the presence of mismatch-induced stress; D and D_S are the coefficients of volumetric and surficial diffusions. Values of dopant diffusions coefficients depends on properties of materials of heterostructure, speed of heating and cooling of materials during annealing and spatio-temporal distribution of concentration of dopant. Dependences of dopant diffusions coefficients on parameters could be approximated by the following relations [23].

$$D_C=D_L(x,y,z,T)\left[1+\xi\frac{\rho^\gamma(x,y,z,t)}{P^\gamma(x,y,z,T)}\right],\ D_S=D_{SL}(x,y,z,T)\left[1+\xi_S\frac{\rho^\gamma(x,y,z,t)}{P^\gamma(x,y,z,T)}\right] \qquad (20)$$

Here $D_L(x, y, z, T)$ and $D_{LS}(x, y, z, T)$ are the spatial (due to accounting all layers of heterostructure) and temperature (due to Arrhenius law) dependences of dopant diffusion coefficients; T is the temperature of annealing; $P(x, y, z, T)$ is the limit of solubility of dopant; parameter γ depends on properties of materials and could be integer in the following interval $\gamma\in$[1, 3, 23]. Concentrational dependence of diffusion coefficients were described in details in [23]. Chemical potential μ in Eq. (19) could be determine by the following relation [24].

$$\mu=E(z)\Omega\sigma_{ij}[u_{ij}(x,y,z,t)+u_{ji}(x,y,z,t)]/2, \qquad (21)$$

where E(z) is the Young modulus, σ_{ij} is the stress tensor; $u_{ij}=\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)$ is the deformation tensor; u_i, u_j are the components $u_x(x, y, z, t)$, $u_y(x, y, z, t)$ and $u_z(x, y, z, t)$ of the displacement vector $\vec{u}(x,y,z,t)$; x_i, x_j are the coordinate x, y, z. The Eq. (21) could be transform to the following form

$$\mu_1(x,y,z,t)=E(z)\frac{\Omega}{2}\left[\frac{\partial u_i(x,y,z,t)}{\partial x_j}+\frac{\partial u_j(x,y,z,t)}{\partial x_i}\right]\left\{\frac{1}{2}\left[\frac{\partial u_i(x,y,z,t)}{\partial x_j}+\frac{\partial u_j(x,y,z,t)}{\partial x_i}\right]-\right.$$

$$-\varepsilon_0\delta_{ij}+\frac{\sigma(z)\delta_{ij}}{1-2\sigma(z)}\left[\frac{\partial u_k(x,y,z,t)}{\partial x_k}-3\varepsilon_0\right]-K(z)\beta(z)[T(x,y,z,t)-T_0]\,\delta_{ij}\Bigg\},$$

$$\mu\,(x,y,z,t)=\left[\frac{\partial u_i(x,y,z,t)}{\partial x_j}+\frac{\partial u_j(x,y,z,t)}{\partial x_i}\right]\left\{\frac{1}{2}\left[\frac{\partial u_i(x,y,z,t)}{\partial x_j}+\frac{\partial u_j(x,y,z,t)}{\partial x_i}\right]-\right.$$

$$\left.-\varepsilon_0\delta_{ij}+\frac{\sigma(z)\delta_{ij}}{1-2\sigma(z)}\left[\frac{\partial u_k(x,y,z,t)}{\partial x_k}-3\varepsilon_0\right]-K(z)\beta(z)[T(x,y,z,t)-T_0]\,\delta_{ij}\right\}\frac{\Omega}{2}E(z),$$

where σ is Poisson coefficient; $\varepsilon_0 = (a_s-a_{EL})/a_{EL}$ is the mismatch parameter; a_s, a_{EL} are lattice distances of the substrate and the epitaxial layer; K is the modulus of uniform compression; β is the coefficient of thermal expansion; T_r is the equilibrium temperature, which coincide (for our case) with room temperature. Components of displacement vector could be obtained by solution of the following equations [24].

$$\begin{cases}\rho\,(z)\dfrac{\partial^2 u_x(x,y,z,t)}{\partial t^2}=\dfrac{\partial\sigma_{xx}(x,y,z,t)}{\partial x}+\dfrac{\partial\sigma_{xy}(x,y,z,t)}{\partial y}+\dfrac{\partial\sigma_{xz}(x,y,z,t)}{\partial z}\\ \rho\,(z)\dfrac{\partial^2 u_y(x,y,z,t)}{\partial t^2}=\dfrac{\partial\sigma_{yx}(x,y,z,t)}{\partial x}+\dfrac{\partial\sigma_{yy}(x,y,z,t)}{\partial y}+\dfrac{\partial\sigma_{yz}(x,y,z,t)}{\partial z}\\ \rho\,(z)\dfrac{\partial^2 u_z(x,y,z,t)}{\partial t^2}=\dfrac{\partial\sigma_{zx}(x,y,z,t)}{\partial x}+\dfrac{\partial\sigma_{zy}(x,y,z,t)}{\partial y}+\dfrac{\partial\sigma_{zz}(x,y,z,t)}{\partial z}\end{cases}$$

Where

$$\sigma_{ij}=\frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial u_i(x,y,z,t)}{\partial x_j}+\frac{\partial u_j(x,y,z,t)}{\partial x_i}-\frac{\delta_{ij}}{3}\frac{\partial u_k(x,y,z,t)}{\partial x_k}\right]+K(z)\delta_{ij}\times$$

$$\times\frac{\partial u_k(x,y,z,t)}{\partial x_k}-\beta(z)K(z)[T(x,y,z,t)-T_r],$$

$\rho\,(z)$ is the density of materials of heterostructure, δ_{ij} Is the Kronecker symbol. With account the relation for σ_{ij} last system of equation could be written as

$$\rho(z)\frac{\partial^2 u_x(x,y,z,t)}{\partial t^2}=\left\{K(z)+\frac{5E(z)}{6[1+\sigma(z)]}\right\}\frac{\partial^2 u_x(x,y,z,t)}{\partial x^2}+\left\{K(z)-\frac{E(z)}{3[1+\sigma(z)]}\right\}\times$$

$$\times\frac{\partial^2 u_y(x,y,z,t)}{\partial x\partial y}+\frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial^2 u_y(x,y,z,t)}{\partial y^2}+\frac{\partial^2 u_z(x,y,z,t)}{\partial z^2}\right]+\left[K(z)+\frac{E(z)}{3[1+\sigma(z)]}\right]\times$$

$$\times\frac{\partial^2 u_z(x,y,z,t)}{\partial x\partial z}-K(z)\beta(z)\frac{\partial T(x,y,z,t)}{\partial x}$$

$$\rho(z)\frac{\partial^2 u_y(x,y,z,t)}{\partial t^2}=\frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial^2 u_y(x,y,z,t)}{\partial x^2}+\frac{\partial^2 u_x(x,y,z,t)}{\partial x\partial y}\right]-\frac{\partial T(x,y,z,t)}{\partial y}\times$$

$$\times K(z)\beta(z)+\frac{\partial}{\partial z}\left\{\frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial u_y(x,y,z,t)}{\partial z}+\frac{\partial u_z(x,y,z,t)}{\partial y}\right]\right\}+\frac{\partial^2 u_y(x,y,z,t)}{\partial y^2}\times$$

(22)

$$\times\left\{\frac{5E(z)}{12[1+\sigma(z)]}+K(z)\right\}+\left\{K(z)-\frac{E(z)}{6[1+\sigma(z)]}\right\}\frac{\partial^2 u_y(x,y,z,t)}{\partial y\partial z}+K(z)\frac{\partial^2 u_y(x,y,z,t)}{\partial x\partial y}$$

$$\rho(z)\frac{\partial^2 u_z(x,y,z,t)}{\partial t^2}=\frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial^2 u_z(x,y,z,t)}{\partial x^2}+\frac{\partial^2 u_z(x,y,z,t)}{\partial y^2}+\frac{\partial^2 u_x(x,y,z,t)}{\partial x\partial z}+\right.$$

$$\left.+\frac{\partial^2 u_y(x,y,z,t)}{\partial y\partial z}\right]+\frac{\partial}{\partial z}\left\{K(z)\left[\frac{\partial u_x(x,y,z,t)}{\partial x}+\frac{\partial u_y(x,y,z,t)}{\partial y}+\frac{\partial u_x(x,y,z,t)}{\partial z}\right]\right\}+$$

$$+\frac{1}{6}\frac{\partial}{\partial z}\left\{\frac{E(z)}{1+\sigma(z)}\left[6\frac{\partial u_z(x,y,z,t)}{\partial z}-\frac{\partial u_x(x,y,z,t)}{\partial x}-\frac{\partial u_y(x,y,z,t)}{\partial y}-\frac{\partial u_z(x,y,z,t)}{\partial z}\right]\right\}-$$

$$-K(z)\beta(z)\frac{\partial T(x,y,z,t)}{\partial z}.$$

Conditions for the system of Eq. (8) could be written in the form

$$\frac{\partial\vec{u}(0,y,z,t)}{\partial x}=0;\quad \frac{\partial\vec{u}(L_x,y,z,t)}{\partial x}=0;\quad \frac{\partial\vec{u}(x,0,z,t)}{\partial y}=0;\quad \frac{\partial\vec{u}(x,L_y,z,t)}{\partial y}=0;$$

$$\frac{\partial\vec{u}(x,y,0,t)}{\partial z}=0;\quad \frac{\partial\vec{u}(x,y,L_z,t)}{\partial z}=0;\quad \vec{u}(x,y,z,0)=\vec{u}_0;\quad \vec{u}(x,y,z,\infty)=\vec{u}_0.$$

Distribution of the concentration of the diffusing substance has been calculated by using of method of averaging of functional corrections. The first-order approximation could be determined by the following relation

$$\rho_1(x,y,z,t)=\alpha_{1C}\Omega\frac{\partial}{\partial x}\int_0^t D_{SL}(x,y,z,T)\nabla_S\mu_1(x,y,z,\tau)\frac{z}{kT}\left[1+\frac{\xi_S\alpha_{1C}^{\gamma}}{P^{\gamma}(x,y,z,T)}\right]d\tau+$$

$$+\alpha_{1C}\Omega\frac{\partial}{\partial y}\int_0^t D_{SL}(x,y,z,T)\nabla_S\mu_1(x,y,z,\tau)\frac{z}{kT}\left[1+\frac{\xi_S\alpha_{1C}^{\gamma}}{P^{\gamma}(x,y,z,T)}\right]d\tau+f_\rho(x,y,z). \quad (19a)$$

Average value of the considered approximation of the considered function could be calculated by using the standard relation [15].

$$\alpha_{1\rho}=\frac{1}{\Theta L_x L_y L_z}\int_0^{\Theta}\int_0^{L_x}\int_0^{L_y}\int_0^{L_z}\rho_1(x,y,z,t)\,d\,z\,d\,y\,d\,x\,d\,t. \quad (23)$$

Substitution of relation (19a) into relation (23) allows obtaining the desired average values in the following form:

$$\alpha_{1\rho}=\frac{1}{L_x L_y L_z}\int_0^{L_x}\int_0^{L_y}\int_0^{L_z}f_\rho(x,y,z)\,d\,z\,d\,y\,d\,x.$$

Next we calculate the second-order approximation of the considered concentration of the diffusant by using the standard iterative procedure of the method of averaging functional corrections [15]. The required approximation was calculated by the following relation

$$\rho_2(x,y,z,t)=\frac{\partial}{\partial z}\int_0^t D_L(x,y,z,T)\frac{\partial \rho_1(x,y,z,\tau)}{\partial z}\left\{1+\xi\frac{[\alpha_{2C}+\rho_1(x,y,z,\tau)]^\gamma}{P^\gamma(x,y,z,T)}\right\}d\tau+$$

$$+f_\rho(x,y,z)+\Omega\frac{\partial}{\partial x}\int_0^t\frac{D_S}{kT}\nabla_S\mu(x,y,z,\tau)\int_0^{L_z}[\alpha_{2\rho}+\rho_1(x,y,W,\tau)]\,dW\,d\tau+$$

$$+\Omega\frac{\partial}{\partial y}\int_0^t\frac{D_S}{kT}\nabla_S\mu(x,y,z,\tau)\int_0^{L_z}[\alpha_{2\rho}+\rho_1(x,y,W,\tau)]\,dW\,d\tau \quad . \tag{19b}$$

The average value of the second approximation of the desired concentration a2r is determined using the standard relation [15] Average value of the second-order approximation of the required concentration $\alpha_{2\rho}$ is determined using the standard relation [15].

$$\alpha_{2\rho}=\frac{1}{\Theta L_xL_yL_z}\int_0^\Theta\int_0^{L_x}\int_0^{L_y}\int_0^{L_z}[\rho_2(x,y,z,t)-\rho_1(x,y,z,t)]\,dz\,dy\,dx\,dt \quad . \tag{24}$$

Substitution of relations (19a) and (19b) into relation (24) gives a possibility to obtain relation for the required average value: $\alpha_{2\rho}$=0. Next let us to solve equations of system (22), i.e. to obtain components of displacement vector. Equations for the first-order approximations of the considered components after appropriate substitution into the Eqs. (22) takes the form

$$\begin{cases}\rho(z)\dfrac{\partial^2 u_{1x}(x,y,z,t)}{\partial t^2}=-K(z)\beta(z)\dfrac{\partial T(x,y,z,t)}{\partial x}\\ \rho(z)\dfrac{\partial^2 u_{1y}(x,y,z,t)}{\partial t^2}=-K(z)\beta(z)\dfrac{\partial T(x,y,z,t)}{\partial y}\\ \rho(z)\dfrac{\partial^2 u_{1z}(x,y,z,t)}{\partial t^2}=-K(z)\beta(z)\dfrac{\partial T(x,y,z,t)}{\partial z}\end{cases} \tag{22a}$$

Integration of the left and right sides of the Eqs. (1b), (3b) and (5b) on time gives us possibility to obtain relations for above approximation in the final form

$$u_{1x}(x,y,z,t)=u_{0x}+K(z)\frac{\beta(z)}{\rho(z)}\frac{\partial}{\partial x}\int_0^t\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta-$$

$$-K(z)\frac{\beta(z)}{\rho(z)}\frac{\partial}{\partial x}\int_0^\infty\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta \quad ,$$

$$u_{1y}(x,y,z,t)=u_{0y}+K(z)\frac{\beta(z)}{\rho(z)}\frac{\partial}{\partial y}\int_0^t\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta-$$

$$-K(z)\frac{\beta(z)}{\rho(z)}\frac{\partial}{\partial y}\int_0^\infty\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta \quad ,$$

$$u_{1z}(x,y,z,t)=u_{0z}+K(z)\frac{\beta(z)}{\rho(z)}\frac{\partial}{\partial z}\int\limits_0^t\int\limits_0^{\vartheta}T(x,y,z,\tau)\,d\tau\,d\vartheta-$$

$$-K(z)\frac{\beta(z)}{\rho(z)}\frac{\partial}{\partial z}\int\limits_0^{\infty}\int\limits_0^{\vartheta}T(x,y,z,\tau)\,d\tau\,d\vartheta.$$

Approximations of the second and higher orders of components of displacement vector could be determined by using standard procedure. The equations for the required components after the standard substitution takes the following form

$$\rho(z)\frac{\partial^2 u_{2x}(x,y,z,t)}{\partial t^2}=\left\{K(z)+\frac{5E(z)}{6[1+\sigma(z)]}\right\}\frac{\partial^2 u_{1x}(x,y,z,t)}{\partial x^2}+\left\{K(z)-\frac{E(z)}{3[1+\sigma(z)]}\right\}\times$$

$$\times\frac{\partial^2 u_{1y}(x,y,z,t)}{\partial x\partial y}+\frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial^2 u_{1y}(x,y,z,t)}{\partial y^2}+\frac{\partial^2 u_{1z}(x,y,z,t)}{\partial z^2}\right]-\frac{\partial T(x,y,z,t)}{\partial x}\times$$

$$\times K(z)\beta(z)+\left\{K(z)+\frac{E(z)}{3[1+\sigma(z)]}\right\}\frac{\partial^2 u_{1z}(x,y,z,t)}{\partial x\partial z}$$

$$\rho(z)\frac{\partial^2 u_{2y}(x,y,z,t)}{\partial t^2}=\frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial^2 u_{1y}(x,y,z,t)}{\partial x^2}+\frac{\partial^2 u_{1x}(x,y,z,t)}{\partial x\partial y}\right]-\frac{\partial T(x,y,z,t)}{\partial y}\times$$

$$\times K(z)\beta(z)+\frac{\partial}{\partial z}\left\{\frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial u_{1y}(x,y,z,t)}{\partial z}+\frac{\partial u_{1z}(x,y,z,t)}{\partial y}\right]\right\}+\frac{\partial^2 u_{1y}(x,y,z,t)}{\partial y^2}\times$$

$$\times\left\{\frac{5E(z)}{12[1+\sigma(z)]}+K(z)\right\}+\left\{K(z)-\frac{E(z)}{6[1+\sigma(z)]}\right\}\frac{\partial^2 u_{1y}(x,y,z,t)}{\partial y\partial z}+K(z)\frac{\partial^2 u_{1y}(x,y,z,t)}{\partial x\partial y}$$

$$\rho(z)\frac{\partial^2 u_{2z}(x,y,z,t)}{\partial t^2}=\frac{E(z)}{2\,[1+\sigma(z)]}\left[\frac{\partial^2 u_{1z}(x,y,z,t)}{\partial x^2}+\frac{\partial^2 u_{1z}(x,y,z,t)}{\partial y^2}+\frac{\partial^2 u_{1x}(x,y,z,t)}{\partial x\partial z}+\right.$$

$$\left.+\frac{\partial^2 u_{1y}(x,y,z,t)}{\partial y\partial z}\right]+\frac{\partial}{\partial z}\left\{K(z)\left[\frac{\partial u_{1x}(x,y,z,t)}{\partial x}+\frac{\partial u_{1y}(x,y,z,t)}{\partial y}+\frac{\partial u_{1x}(x,y,z,t)}{\partial z}\right]\right\}+$$

$$+\frac{E(z)}{6[1+\sigma(z)]}\frac{\partial}{\partial z}\left[6\frac{\partial u_{1z}(x,y,z,t)}{\partial z}-\frac{\partial u_{1x}(x,y,z,t)}{\partial x}-\frac{\partial u_{1y}(x,y,z,t)}{\partial y}-\frac{\partial u_{1z}(x,y,z,t)}{\partial z}\right]-$$

$$\left.\left.-\frac{\partial u_{1x}(x,y,z,t)}{\partial x}-\frac{\partial u_{1y}(x,y,z,t)}{\partial y}-\frac{\partial u_{1z}(x,y,z,t)}{\partial z}\right]\right\}\frac{E(z)}{1+\sigma(z)}-K(z)\beta(z)\frac{\partial T(x,y,z,t)}{\partial z}.$$

Integration of the left and right sides of the above relations on time *t* leads to the following result

$$u_{2x}(x,y,z,t)=\frac{1}{\rho(z)}\left\{K(z)+\frac{5E(z)}{6[1+\sigma(z)]}\right\}\frac{\partial^2}{\partial x^2}\int_0^t\int_0^{\vartheta}u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{1}{\rho(z)}\left\{K(z)-\right.$$

$$\left.-\frac{E(z)}{3[1+\sigma(z)]}\right\}\frac{\partial^2}{\partial x\partial y}\int_0^t\int_0^{\vartheta}u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{E(z)}{2\rho(z)}\left[\frac{\partial^2}{\partial y^2}\int_0^t\int_0^{\vartheta}u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta+\right.$$

$$\left.+\frac{\partial^2}{\partial z^2}\int_0^t\int_0^{\vartheta}u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta\right]\frac{1}{1+\sigma(z)}+\frac{1}{\rho(z)}\frac{\partial^2}{\partial x\partial z}\int_0^t\int_0^{\vartheta}u_{1z}(x,y,z,\tau)d\tau\,d\vartheta\left\{K(z)+\right.$$

$$\left.+\frac{E(z)}{3[1+\sigma(z)]}\right\}-K(z)\frac{\beta(z)}{\rho(z)}\frac{\partial}{\partial x}\int_0^t\int_0^{\vartheta}T(x,y,z,\tau)\,d\tau\,d\vartheta-\frac{\partial^2}{\partial x^2}\int_0^{\infty}\int_0^{\vartheta}u_{1x}(x,y,z,\tau)d\tau\,d\vartheta\times$$

$$\times\frac{1}{\rho(z)}\left\{K(z)+\frac{5E(z)}{6[1+\sigma(z)]}\right\}-\left\{K(z)-\frac{E(z)}{3[1+\sigma(z)]}\right\}\frac{\partial^2}{\partial x\partial y}\int_0^{\infty}\int_0^{\vartheta}u_{1y}(x,y,z,\tau)d\tau\,d\vartheta\times$$

$$\times\frac{1}{\rho(z)}-\frac{E(z)}{2\rho(z)[1+\sigma(z)]}\left[\frac{\partial^2}{\partial y^2}\int_0^{\infty}\int_0^{\vartheta}u_{1y}(x,y,z,\tau)d\tau\,d\vartheta+\frac{\partial^2}{\partial z^2}\int_0^{\infty}\int_0^{\vartheta}u_{1z}(x,y,z,\tau)d\tau\,d\vartheta\right]-$$

$$-\frac{1}{\rho(z)}\left\{K(z)+\frac{E(z)}{3[1+\sigma(z)]}\right\}\frac{\partial^2}{\partial x\partial z}\int_0^{\infty}\int_0^{\vartheta}u_{1z}(x,y,z,\tau)d\tau\,d\vartheta+u_{0x}+K(z)\frac{\beta(z)}{\rho(z)}\times$$

$$\times\frac{\partial}{\partial x}\int_0^{\infty}\int_0^{\vartheta}T(x,y,z,\tau)\,d\tau\,d\vartheta$$

$$u_{2y}(x,y,z,t)=\frac{E(z)}{2\rho(z)}\left[\frac{\partial^2}{\partial x^2}\int_0^t\int_0^{\vartheta}u_{1x}(x,y,z,\tau)d\tau\,d\vartheta+\frac{\partial^2}{\partial x\partial y}\int_0^t\int_0^{\vartheta}u_{1x}(x,y,z,\tau)d\tau\,d\vartheta\right]\times$$

$$\times\frac{1}{1+\sigma(z)}+\frac{K(z)}{\rho(z)}\frac{\partial^2}{\partial x\partial y}\int_0^t\int_0^{\vartheta}u_{1y}(x,y,z,\tau)d\tau\,d\vartheta+\frac{1}{\rho(z)}\left\{\frac{5E(z)}{12[1+\sigma(z)]}+K(z)\right\}\times$$

$$\times\frac{\partial^2}{\partial y^2}\int_0^t\int_0^{\vartheta}u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{1}{2\rho(z)}\frac{\partial}{\partial z}\left\{\frac{E(z)}{1+\sigma(z)}\left[\frac{\partial}{\partial z}\int_0^t\int_0^{\vartheta}u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta+\right.\right.$$

$$\left.\left.+\frac{\partial}{\partial y}\int_0^t\int_0^{\vartheta}u_{1z}(x,y,z,\tau)d\tau\,d\vartheta\right]\right\}-K(z)\frac{\beta(z)}{\rho(z)}\int_0^t\int_0^{\vartheta}T\,(x,y,z,\tau)d\tau\,d\vartheta-\left\{\frac{E(z)}{6[1+\sigma(z)]}-\right.$$

$$\left.-K(z)\right\}\frac{1}{\rho(z)}\frac{\partial^2}{\partial y\partial z}\int_0^t\int_0^{\vartheta}u_{1y}(x,y,z,\tau)d\tau\,d\vartheta-\frac{E(z)}{2\rho(z)}\left[\frac{\partial^2}{\partial x^2}\int_0^{\infty}\int_0^{\vartheta}u_{1x}(x,y,z,\tau)d\tau\,d\vartheta+\right.$$

$$+\frac{\partial^2}{\partial x \partial y}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)d\tau d\vartheta\right]\frac{1}{1+\sigma(z)}-K(z)\frac{\beta(z)}{\rho(z)}\int_0^\infty\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta-\frac{K(z)}{\rho(z)}\times$$

$$\times\frac{\partial^2}{\partial x \partial y}\int_0^\infty\int_0^\vartheta u_{1y}(x,y,z,\tau)d\tau d\vartheta-\frac{1}{\rho(z)}\frac{\partial^2}{\partial y^2}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta\left\{\frac{5E(z)}{12[1+\sigma(z)]}+\right.$$

$$\left.+K(z)\right\}-\frac{\partial}{\partial z}\left\{\frac{E(z)}{1+\sigma(z)}\left[\frac{\partial}{\partial z}\int_0^\infty\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{\partial}{\partial y}\int_0^\infty\int_0^\vartheta u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta\right]\right\}\times$$

$$\times\frac{1}{2\rho(z)}-\frac{1}{\rho(z)}\left\{K(z)-\frac{E(z)}{6[1+\sigma(z)]}\right\}\frac{\partial^2}{\partial y \partial z}\int_0^\infty\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta+u_{0y}$$

$$u_z(x,y,z,t)=\frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial^2}{\partial x^2}\int_0^\infty\int_0^\vartheta u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{\partial^2}{\partial y^2}\int_0^\infty\int_0^\vartheta u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta+\right.$$

$$\left.+\frac{\partial^2}{\partial x \partial z}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{\partial^2}{\partial y \partial z}\int_0^\infty\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta\right]\frac{1}{\rho(z)}+\frac{1}{\rho(z)}\times$$

$$\times\frac{\partial}{\partial z}\left\{K(z)\left[\frac{\partial}{\partial x}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{\partial}{\partial y}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta+\right.\right.$$

$$\left.\left.+\frac{\partial}{\partial z}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta\right]\right\}+\frac{1}{6\rho(z)}\frac{\partial}{\partial z}\left\{\frac{E(z)}{1+\sigma(z)}\left[6\frac{\partial}{\partial z}\int_0^\infty\int_0^\vartheta u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta-\right.\right.$$

$$\left.\left.-\frac{\partial}{\partial x}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta-\frac{\partial}{\partial y}\int_0^\infty\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta-\frac{\partial}{\partial z}\int_0^\infty\int_0^\vartheta u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta\right]\right\}-$$

$$-K(z)\frac{\beta(z)}{\rho(z)}\frac{\partial}{\partial z}\int_0^\infty\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta+u_{0z}$$

.

In this paper we calculate concentrations of a mixture of gases and a diffusing materials in the considered heterostructure, distribution of temperature and components of displacement vector as the second-order approximations framework the method of averaging functional corrections. This approximation is usually enough good for obtaining qualitative conclusions and obtaining some quantitative results. The results of analytical calculations were verified by comparison them with results of numerical simulation.

Discussion

In this section we analyzed the diffusion mixing of the heterostructure layers during annealing with account the relaxation of miss match-induced stresses. Typical distributions of diffusant concentrations in the considered heterostructure are shown in Fig. 2 for different continuance of annealing time. The conclusions in this case are standard: an increase in the duration of annealing leads to a more homogenous distribution of the diffusant. At the same time mixing of heterostructure materials leads to decreasing in mechanical stresses (see Fig. 3). It should be noted that the porosity of the buffer layer leads to increasing this effect.

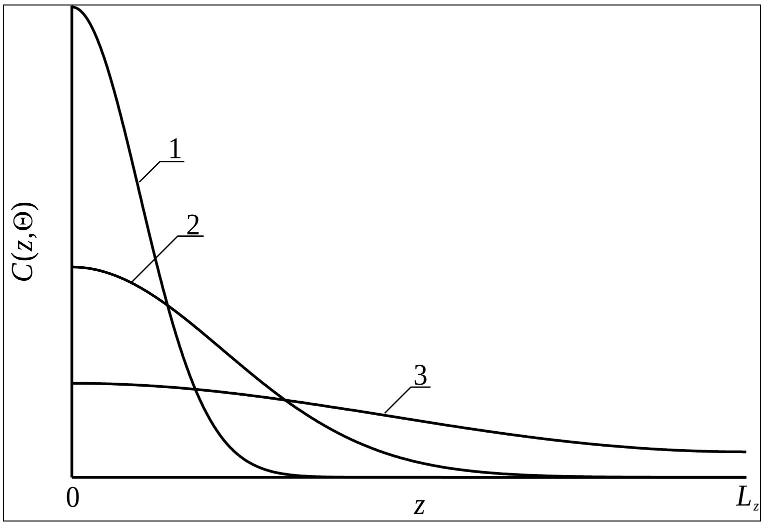

Fig 2: Spatial distributions of diffusant in the considered heterostructure at different values of continuance of annealing time. Increasing of number of curves corresponds to increasing of continuance of annealing time.

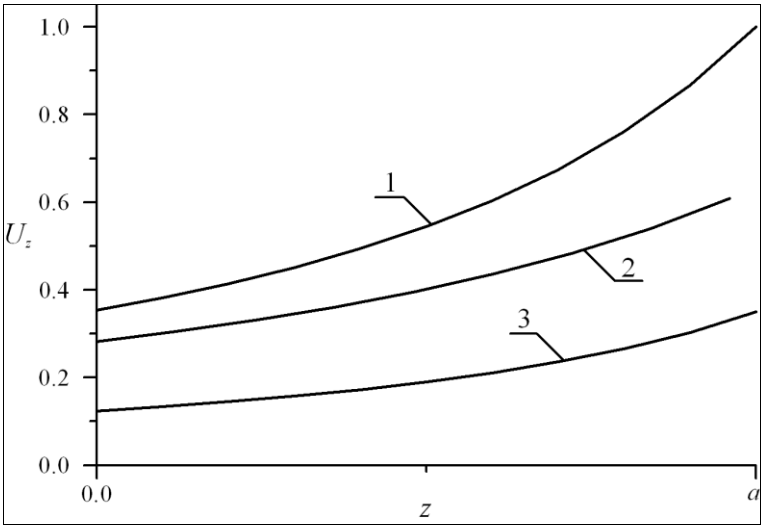

Fig 3: Normalized dependences of the component of the displacement vector u_z on the *z* coordinate (a is the thickness of the buffer layer). Increasing of number of curves corresponds to increasing of continuance of annealing time

Conclusion

In this paper we analyzed the effect of processing the substrate, which precedes the growth of new epitaxial layers, on properties of the grown heterostructure. It has been shown, that growth of the new epitaxial layer on the buffer layer after preliminary (before the start of growth) annealing reduces the value of miss match-induced stresses. An analytical approach has been introduced for analysis of mass and heat transfer in a multilayer structures with account miss match-induced stress.

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