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On prognosis of variation of properties of multilayer structure by preliminary processing of the substrate

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ABSTRACT

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

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1. INTRODUCTION

To manufacture 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 use of heterostructures in different devices were described in a large number of experimental works [1]–[11]. At the same time, fewer works are describing the prediction of epitaxy processes [12], [13]. In this paper, we consider a vertical reactor for gas phase epitaxy as presented in Figure 1. The reactor consists of an external casing, a substrate holder with a substrate, and a spiral around the casing in the area of the substrate to generate induction heating to activate chemical reactions of decay of reagents and to the growth of the epitaxial layer.

A gaseous mixture of reagents together with gas-carrier inputs into the 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 obtained structure was annealed. After that an epitaxial layer was grown on the buffer layer. The main aim of this paper was analyzed of changing of the properties of the final heterostructure under influence of the considered annealing after grown of the buffer layer. Additionally, we introduce 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, mismatch-induced stresses.

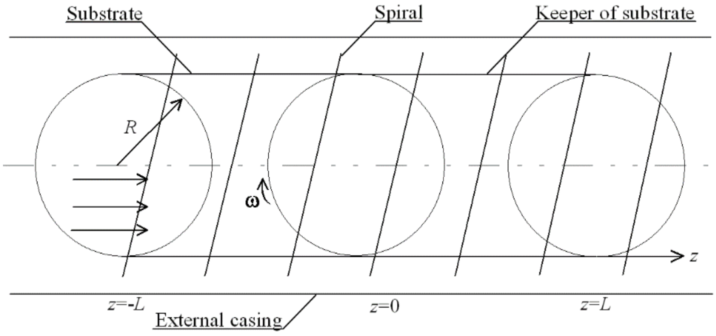

Figure 1. A reactor for the gas phase epitaxy in neighborhoods of the reaction zone

2. METHOD OF SOLUTION

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

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

Where the vector $\vec{v}$ is the speed of flow of the considered mixture of gases; parameter c is the capacity of heat; function $T(r,\varphi,z,t)$ is the distribution of temperature in space and time; function $p(r,\varphi,z,t)$ describes the power density, which stands out in the considered system substrate - keeper; r, φ and z are the cylindrical coordinates; t is the current time; function $C(r,\varphi,z,t)$ describes the distribution of concentration of mixture of gases in space and time; parameter λ describes the conductivity of heat. The value of heat conductivity could be determined by the relation: $\lambda = \bar{v}\bar{l}c_v\rho/3$, where $\bar{v}$ is the modulus of the 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 the gas.

To solve this boundary problem, one shall take into account the moving of a mixture of gases and the 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 the radius of the keeper of substrate R is essentially larger than the 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 (2) and (3).

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

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

Where D is the diffusion coefficient of a 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 (4).

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

$$C(0,\varphi,z,t) \neq \infty,\ \left.\frac{\partial C(r,\phi,z,t)}{\partial r}\right|_{r=R} = 0,\ \left.\frac{\partial C(r,\phi,z,t)}{\partial \phi}\right|_{\phi=0} = \left.\frac{\partial C(r,\phi,z,t)}{\partial \phi}\right|_{\phi=2\pi},\ T(r,\varphi,z,0) = T_r,$$
$$-\lambda\left.\frac{\partial T(r,\phi,z,t)}{\partial r}\right|_{r=R} = \sigma T^4(R,\phi,z,t),\ \left.\frac{\partial T(r,\phi,z,t)}{\partial \phi}\right|_{\phi=0} = \left.\frac{\partial T(r,\phi,z,t)}{\partial \phi}\right|_{\phi=2\pi},$$
$$-\lambda\left.\frac{\partial T(r,\phi,z,t)}{\partial z}\right|_{z=-L} = \sigma T^4(r,\phi,-L,t),\ T(r,0,z,t) = T(r,2\pi,z,t),\ \left.\frac{\partial v_r(r,\phi,z,t)}{\partial r}\right|_{r=0} = 0,$$
$$\left.\frac{\partial v_\phi(r,\phi,z,t)}{\partial \phi}\right|_{\phi=0} = \left.\frac{\partial v_\phi(r,\phi,z,t)}{\partial \phi}\right|_{\phi=2\pi},\ \left.\frac{\partial v_\phi(r,\phi,z,t)}{\partial \phi}\right|_{\phi=0} = \left.\frac{\partial v_\phi(r,\phi,z,t)}{\partial \phi}\right|_{\phi=2\pi}, \qquad (4)$$

$\left.\frac{\partial v_r(r,\phi,z,t)}{\partial r}\right|_{r=R} = 0$, $-\lambda\left.\frac{\partial T(r,\phi,z,t)}{\partial z}\right|_{z=L} = \sigma T^4(r,\phi,z,t)$, $T(0,\varphi,z,t) \neq \infty$, $v_r(r,\varphi,-L,t) = 0$,
$v_r(r,\varphi,0,t) = 0$, $v_r(r,\varphi,L,t) = 0$, $v_r(r,0,z,t) = v_r(r,2\pi,z,t)$, $v_r(0,\varphi,z,t) \neq \infty$, $v_\varphi(r,\varphi,0,t) = \omega r$,
$v_\varphi(r,\varphi,-L,t) = 0$, $v_\varphi(r,\varphi,L,t) = 0$, $v_\varphi(r,0,z,t) = v_\varphi(r,2\pi,z,t)$, $v_\varphi(0,\varphi,z,t) \neq \infty$, $v_z(r,\varphi,-L,t) = V_0$,
$v_z(r,\varphi,0,t) = \bar{v}_z$, $v_z(r,\varphi,L,t) = 0$, $v_z(r,0,z,t) = v_z(r,2\pi,z,t)$, $v_z(0,\varphi,z,t) \neq \infty$, $v_r(r,\varphi,z,0) = 0$,
$v_\varphi(r,\varphi,z,0) = 0$, $v_z(r,\varphi,-L,0) = V_0$.

Here parameter σ is equal to $\sigma = 5.67.10^{-8}$ $W.m^{-2}.K^{-4}$, parameter T_r describes the room temperature, parameter ω describes the frequency of rotation of the substrate. Equations for components of velocity of flow with account cylindrical system of coordinate could be written as (5a)-(5c).

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

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

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

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

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

Solutions to the above equations could be written as (7).

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

The second-order approximations of components of the speed of flow could be obtained by replacement of the required functions on the following sums $v_r \rightarrow \alpha_{1r}$, $v_\varphi \rightarrow \alpha_{1\varphi}$, $v_z \rightarrow \alpha_{1z}$. Approximations for the components could be written as (8a)-(8c).

$$\begin{aligned}\frac{\partial v_{2r}}{\partial t} &= \nu\left(\frac{\partial^2 v_{1r}}{\partial r^2} + \frac{\partial^2 v_{1r}}{\partial r\partial z} - \frac{\partial^2 v_{1r}}{\partial z^2} + \frac{\partial^2 v_{1z}}{\partial r\partial z}\right) - \frac{\partial}{\partial r}\left(\frac{P}{\xi}\right) - (\alpha_{2r} + v_{1r})\frac{\partial v_{1r}}{\partial r} - \frac{(\alpha_{2\phi}+v_{1\phi})}{r}\frac{\partial v_{1r}}{\partial \phi}\\ &-(\alpha_{2z} + v_{1z})\frac{\partial v_{1r}}{\partial z},\end{aligned} \tag{8a}$$

$$\begin{aligned}\frac{\partial v_{2\phi}}{\partial t} &= \nu\left(\frac{1}{r}\frac{\partial^2 v_{1r}}{\partial r\partial \phi} + \frac{2}{r^2}\frac{\partial^2 v_{1\phi}}{\partial \phi^2} - \frac{1}{r^2}\frac{\partial^2 v_{1r}}{\partial \phi\partial z} + \frac{\partial^2 v_{1\phi}}{\partial z^2}\right) - \frac{1}{r}\frac{\partial}{\partial \phi}\left(\frac{P}{\xi}\right) - (\alpha_{2r} + v_{1r})\frac{\partial v_{1\phi}}{\partial r}\\ &- \frac{(\alpha_{2\phi}+v_{1\phi})}{r}\frac{\partial v_{1\phi}}{\partial \phi} - (\alpha_{2z} + v_{1z})\frac{\partial v_{1\phi}}{\partial z},\end{aligned} \tag{8b}$$

$$\begin{aligned}\frac{\partial v_{2z}}{\partial t} &= \nu\left(\frac{\partial^2 v_{1r}}{\partial z^2} + \frac{\partial^2 v_{1z}}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 v_{1z}}{\partial \phi^2}\right) - \frac{\partial}{\partial z}\left(\frac{P}{\xi}\right) - (\alpha_{2r} + v_{1r})\frac{\partial v_{1z}}{\partial r} - \frac{(\alpha_{2\phi}+v_{1\phi})}{r}\frac{\partial v_{1z}}{\partial \phi}\\ &-(\alpha_{2z} + v_{1z})\frac{\partial v_{1z}}{\partial z}\end{aligned} \tag{8c}$$

Integration of the above equations leads to the following result.

$$\begin{aligned}v_{2r} &= \nu\int_0^t\left(\frac{\partial^2 v_{1r}}{\partial r^2} + \frac{\partial^2 v_{1r}}{\partial r\partial z} - \frac{\partial^2 v_{1r}}{\partial z^2} + \frac{\partial^2 v_{1z}}{\partial r\partial z}\right)d\tau - \frac{\partial}{\partial r}\left(\int_0^t \frac{P}{\xi}d\tau\right) - \int_0^t(\alpha_{2r} + v_{1r})\frac{\partial v_{1r}}{\partial r}d\tau\\ &- \int_0^t \frac{(\alpha_{2\phi}+v_{1\phi})}{r}\frac{\partial v_{1r}}{\partial \phi}d\tau - \int_0^t(\alpha_{2z} + v_{1z})\frac{\partial v_{1r}}{\partial z}d\tau,\end{aligned} \tag{8d}$$

$$\begin{aligned}v_{2\phi} &= \nu\int_0^t\left(\frac{1}{r}\frac{\partial^2 v_{1r}}{\partial r\partial \phi} + \frac{2}{r^2}\frac{\partial^2 v_{1\phi}}{\partial \phi^2} - \frac{1}{r^2}\frac{\partial^2 v_{1r}}{\partial \phi\partial z} + \frac{\partial^2 v_{1\phi}}{\partial z^2}\right)d\tau - \frac{1}{r}\frac{\partial}{\partial \phi}\left(\int_0^t \frac{P}{\xi}d\tau\right)\\ &- \int_0^t(\alpha_{2r} + v_{1r})\frac{\partial v_{1\phi}}{\partial r}d\tau - \int_0^t \frac{(\alpha_{2\phi}+v_{1\phi})}{r}\frac{\partial v_{1\phi}}{\partial \phi}d\tau - \int_0^t(\alpha_{2z} + v_{1z})\frac{\partial v_{1\phi}}{\partial z}d\tau,\end{aligned} \tag{8e}$$

$$v_{2z} = \nu \int_0^t \left(\frac{\partial^2 v_{1r}}{\partial z^2} + \frac{\partial^2 v_{1z}}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 v_{1z}}{\partial \phi^2}\right) d\tau - \frac{\partial}{\partial z}\left(\int_0^t \frac{P}{\xi} d\tau\right) - \int_0^t (\alpha_{2r} + v_{1r}) \frac{\partial v_{1z}}{\partial r} d\tau - \int_0^t \frac{(\alpha_{2\phi}+v_{1\phi})}{r} \left(\alpha_{2\phi} + v_{1\phi}\right) \frac{\partial v_{1z}}{\partial \phi} d\tau - \int_0^t (\alpha_{2z} + v_{1z}) \frac{\partial v_{1z}}{\partial z} d\tau \tag{8f}$$

We determine average values α_{2r}, $\alpha_{2\varphi}$, α_{2z} by (9).

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

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

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

Where Θ is the continuance of moving of the mixture of gases through the reactor? Substitution of the first and second-order approximations of the required components of speed into the relation (9) give us the possibility to obtain a system of equations to determine required average values.

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

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

The solution of the above system of equations could be determined by standard approaches [21] and could be written as (11).

$$\alpha_{2r} = \Delta_r / \Delta,\ \alpha_{2\phi} = \Delta_\phi / \Delta,\ \alpha_{2z} = \Delta_z / \Delta, \tag{11}$$

Where $\Delta = A_1 (B_2 C_3 - B_3 C_2) - B_1 (A_2 C_3 - A_3 C_2) + C_1 (A_2 B_3 - A_3 B_2)$, $\Delta_r = D_1 (B_2 C_3 - B_3 C_2) -$
$- B_1 (D_2 C_3 - D_3 C_2) + C_1 (D_2 B_3 - D_3 B_2)$, $\Delta_\phi = D_1 (B_2 C_3 - B_3 C_2) - B_1 (D_2 C_3 - D_3 C_2) + C_1 \times$
$\times (D_2 B_3 - D_3 B_2)$, $\Delta_z = A_1 (B_2 D_3 - B_3 D_2) - B_1 (A_2 D_3 - A_3 D_2) + D_1 (A_2 B_3 - A_3 B_2)$.

In this section, we obtained components of velocity of the stream of a mixture of materials in the gas phase, which are used for the growth of heterostructure, and gas-carrier in the second-order approximation framework method of averaging function corrections. Usually, the second-order approximation is enough good approximation to make a qualitative analysis of obtained solution and to obtain some quantitative results. Let us rewrite (1) and (3) by using a cylindrical system of coordinates.

$$c \frac{\partial T(r,\phi,z,t)}{\partial t} = \lambda \left[\frac{\partial^2 T(r,\phi,z,t)}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 T(r,\phi,z,t)}{\partial \phi^2} + \frac{\partial^2 T(r,\phi,z,t)}{\partial z^2}\right] - c \cdot \frac{\partial}{\partial r}\{C(r,\phi,z,t) \cdot T(r,\phi,z,t) \cdot [v_r(r,\phi,z,t) - \bar{v}_r(r,\phi,z,t)]\} - \frac{c}{r}\frac{\partial}{\partial \phi}\{\left[v_\phi(r,\phi,z,t) - \bar{v}_\phi(r,\phi,z,t)\right] \cdot C(r,\phi,z,t) \cdot T(r,\phi,z,t)\} - c \cdot \frac{\partial}{\partial z}\{[v_z(r,\phi,z,t) - \bar{v}_z(r,\phi,z,t)] \cdot C(r,\phi,z,t) \cdot T(r,\phi,z,t)\} + p(r,\phi,z,t) \tag{12}$$

$$\frac{\partial C(r,\phi,z,t)}{\partial t}=\frac{1}{r}\frac{\partial}{\partial r}\left[rD\frac{\partial C(r,\phi,z,t)}{\partial r}\right]+\frac{1}{r^2}\frac{\partial}{\partial \phi}\left[D\frac{\partial C(r,\phi,z,t)}{\partial \phi}\right]+\frac{\partial}{\partial z}\left[D\frac{\partial C(r,\phi,z,t)}{\partial z}\right]-\frac{1}{r}\frac{\partial}{\partial r}\{rC(r,\phi,z,t)\cdot [v_r(r,\phi,z,t)-\bar{v}_r(r,\phi,z,t)]\}-\frac{1}{r}\frac{\partial}{\partial \phi}\{rC(r,\phi,z,t)\cdot\left[v_\phi(r,\phi,z,t)-\bar{v}_\phi(r,\phi,z,t)\right]\}-\frac{\partial}{\partial z}\{C(r,\phi,z,t)\cdot[v_z(r,\phi,z,t)-\bar{v}_z(r,\phi,z,t)]\}. \tag{13}$$

We calculate the distribution of temperature in space and time and the same distribution of concentration of the mixture of gases we used the method of an 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} on the right sides of the above equations. Further, we used a recently consider algorithm to obtain the first-order approximations of the temperature and concentration of the gas mixture.

$$T_1(r,\phi,z,t)=T_r+\int_0^t\frac{p(r,\phi,z,\tau)}{c}d\tau-\alpha_{1T}\alpha_{1C}\int_0^t\frac{\partial[v_r(r,\phi,z,\tau)-\bar{v}_r(r,\phi,z,\tau)]}{\partial r}d\tau-\frac{\alpha_{1T}\alpha_{1C}}{r}\int_0^t\frac{\partial[v_\phi(r,\phi,z,\tau)-\bar{v}_\phi(r,\phi,z,\tau)]}{\partial\phi}d\tau-\alpha_{1T}\alpha_{1C}\int_0^t\frac{\partial[v_z(r,\phi,z,\tau)-\bar{v}_z(r,\phi,z,\tau)]}{\partial z}d\tau \tag{14}$$

$$C_1(r,\phi,z,t)=C_0-\frac{\alpha_{1C}}{r}\int_0^t\frac{\partial\{r[v_r(r,\phi,z,\tau)-\bar{v}_r(r,\phi,z,\tau)]\}}{\partial r}d\tau-\frac{\alpha_{1C}}{r}\int_0^t\frac{\partial[v_\phi(r,\phi,z,\tau)-\bar{v}_\phi(r,\phi,z,\tau)]}{\partial\phi}d\tau-\alpha_{1C}\int_0^t\frac{\partial[v_z(r,\phi,z,\tau)-\bar{v}_z(r,\phi,z,\tau)]}{\partial z}d\tau \tag{15}$$

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

$$\alpha_{1T}=\frac{1}{\pi\Theta R^2L}\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^L T_1(r,\phi,z,\tau)dzd\phi drdt,$$
$$\alpha_{1C}=\frac{1}{\pi\Theta R^2L}\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^L C_1(r,\phi,z,\tau)dzd\phi drdt. \tag{16}$$

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

$$\alpha_{1C}=C_0/L\cdot\left\{1+\frac{1}{\pi\Theta RL}\int_0^\Theta(\Theta-t)\int_0^{2\pi}\int_{-L}^L[v_r(R,\phi,z,t)-\bar{v}_r(R,\phi,z,t)]dzd\phi dt+\frac{\Theta V_0}{RL}\right\},$$
$$\alpha_{1T}=\left[T_r+\frac{1}{\pi\Theta R^2L}\int_0^\Theta(\Theta-t)\int_0^R r\int_0^{2\pi}\int_{-L}^L\frac{p(r,\phi,z,t)}{c}dzd\phi drdt\right]\left(1+\frac{C_0}{\pi\Theta RL^2}\left\{\int_0^\Theta(\Theta-t)\times\right.\right.$$
$$\times\int_0^{2\pi}\int_{-L}^L[v_r(R,\phi,z,\tau)-\bar{v}_r(R,\phi,z,\tau)]dzd\phi dt-\int_0^\Theta\int_0^R\int_0^{2\pi}\int_{-L}^L[v_r(r,\phi,z,t)-\bar{v}_r(r,\phi,z,t)]dzd\phi dr\times(\Theta-t)dt\frac{1}{\pi\Theta R^2}+\frac{V_0}{2}\right\}\left\{\frac{1}{\pi\Theta RL}\int_0^\Theta(\Theta-t)\int_0^{2\pi}\int_{-L}^L[v_r(R,\phi,z,\tau)-\bar{v}_r(R,\phi,z,\tau)]dzd\phi dt+1+\Theta V_0/RL\right\}^{-1}\Bigg)$$

The second-order approximations of temperature and concentration of the mixture of gases we determine the framework for the method of averaging of function corrections [15]–[20], i.e. by replacement of the required functions on the right sides of (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 (17a) and (17b).

$$c\cdot T_2(r,\phi,z,t)=\lambda\int_0^t\frac{\partial^2T_1(r,\phi,z,\tau)}{\partial r^2}d\tau+\lambda\frac{1}{r^2}\int_0^t\frac{\partial^2T_1(r,\phi,z,\tau)}{\partial\phi^2}d\tau+\lambda\int_0^t\frac{\partial^2T_1(r,\phi,z,\tau)}{\partial z^2}d\tau+$$
$$-c\cdot\frac{\partial}{\partial r}\int_0^t\{[v_r(r,\phi,z,\tau)-\bar{v}_r(r,\phi,z,\tau)]\cdot[\alpha_{2C}+C_1(r,\phi,z,\tau)]\cdot[\alpha_{2T}+T_1(r,\phi,z,\tau)]\}d\tau$$
$$-\frac{c}{r}\frac{\partial}{\partial\phi}\int_0^t\{[\alpha_{2C}+C_1(r,\phi,z,\tau)]\cdot\left[v_\phi(r,\phi,z,\tau)-\bar{v}_\phi(r,\phi,z,\tau)\right]\cdot[\alpha_{2T}+T_1(r,\phi,z,\tau)]\}d\tau$$
$$-c\cdot\frac{\partial}{\partial z}\int_0^t\{[v_z(r,\phi,z,\tau)-\bar{v}_z(r,\phi,z,\tau)]\cdot[\alpha_{2C}+C_1(r,\phi,z,\tau)]\cdot[\alpha_{2T}+T_1(r,\phi,z,\tau)]\}d\tau$$
$$+\int_0^t p(r,\phi,z,\tau)d\tau+T_r, \tag{17a}$$

$$C_2(r,\phi,z,t)=\frac{1}{r}\frac{\partial}{\partial r}\int_0^t rD\frac{\partial C_1(r,\phi,z,\tau)}{\partial r}d\tau+\frac{1}{r^2}\frac{\partial}{\partial\phi}\int_0^t D\frac{\partial C_1(r,\phi,z,\tau)}{\partial\phi}d\tau+\frac{\partial}{\partial z}\int_0^t D\frac{\partial C_1(r,\phi,z,\tau)}{\partial z}d\tau$$
$$-\frac{1}{r}\frac{\partial}{\partial r}\left\{r\int_0^t[\alpha_{2C}+C_1(r,\phi,z,\tau)]\cdot[v_r(r,\phi,z,\tau)-\bar{v}_r(r,\phi,z,\tau)]d\tau\right\}$$
$$-\frac{1}{r}\frac{\partial}{\partial\phi}\int_0^t[\alpha_{2C}+C_1(r,\phi,z,\tau)]\cdot\left[v_\phi(r,\phi,z,\tau)-\bar{v}_\phi(r,\phi,z,\tau)\right]d\tau+C_0\delta(z+L)$$
$$-\frac{\partial}{\partial z}\int_0^t[\alpha_{2C}+C_1(r,\phi,z,\tau)]\cdot[v_z(r,\phi,z,\tau)-\bar{v}_z(r,\phi,z,\tau)]d\tau. \tag{17b}$$

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

$$\alpha_{2T}=\frac{1}{\pi\Theta R^2L}\int_0^{\Theta}\int_0^{R}r\int_0^{2\pi}\int_{-L}^{L}(T_2-T_1)dzd\phi drdt,$$

$$\alpha_{2C}=\frac{1}{\pi\Theta R^2L}\int_0^{\Theta}\int_0^{R}r\int_0^{2\pi}\int_{-L}^{L}(C_2-C_1)dzd\phi drdt. \tag{18}$$

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

$$\alpha_{2T}=\left(\frac{\lambda\sigma}{c\pi\Theta RL}\int_0^{\Theta}(\Theta-t)\int_0^{2\pi}\int_{-L}^{L}T^4(R,\phi,z,t)dzd\phi dt-\int_0^{\Theta}(\Theta-\right.$$
$$t)\int_0^{2\pi}\int_{-L}^{L}T_1(R,\phi,z,t)dzd\phi dt\times\frac{\lambda}{c\pi\Theta R^2L}+\frac{\lambda}{c\pi\Theta R^2L}\int_0^{\Theta}(\Theta-t)\int_0^{2\pi}\int_{-L}^{L}T_1(0,\phi,z,t)dzd\phi dt-$$
$$\int_0^{\Theta}(\Theta-t)\int_0^{2\pi}\int_{-L}^{L}\{T_1(R,\phi,z,t)\times[\alpha_{2C}+C_1(R,\phi,z,t)]-\alpha_{1T}\alpha_{1C}\}[v_r(R,\phi,z,t)-$$
$$\bar{v}_r(R,\phi,z,t)]dzd\phi dt\frac{1}{\pi\Theta RL}-\frac{1}{\pi\Theta R^2L}\times\int_0^{\Theta}\int_0^{R}r\int_0^{2\pi}\int_{-L}^{L}\{T_1(r,\phi,z,t)[\alpha_{2C}+C_1(r,\phi,z,t)]-\alpha_{1T}\alpha_{1C}\}\cdot$$
$$[v_r(r,\phi,z,t)-\bar{v}_r(r,\phi,z,t)]dzd\phi dr\times(\Theta-t)dt-\frac{V_0}{\pi\Theta R^2L}\int_0^{\Theta}(\Theta-t)\int_0^{R}r\int_0^{2\pi}[T_1(r,\phi,L,t)(\alpha_{2C}+$$
$$C_0)-\alpha_{1T}\alpha_{1C}]d\phi drdt\left\{\frac{1}{\pi\Theta RL}\times\int_0^{\Theta}(\Theta-t)\int_0^{2\pi}\int_{-L}^{L}[v_r(R,\phi,z,t)-\bar{v}_r(R,\phi,z,t)][\alpha_{2C}+\right.$$
$$C_1(R,\phi,z,t)]dzd\phi dt+1-\frac{1}{\pi\Theta R^2L}\times\int_0^{\Theta}(\Theta-t)\int_0^{R}r\int_0^{2\pi}\int_{-L}^{L}[v_r(r,\phi,z,t)-\bar{v}_r(r,\phi,z,t)]\cdot$$
$$\left.[\alpha_{2C}+C_1(r,\phi,z,t)]dzd\phi drdt+(\alpha_{2C}+C_0)\times+2\Theta V_0/L\right\}^{-1},$$

$$\alpha_{2C}=\frac{1}{\pi\Theta R^2L}\int_0^{\Theta}(\Theta-t)\int_0^{R}r\int_0^{2\pi}D\left[\left.\frac{\partial C_1(r,\phi,z,\tau)}{\partial z}\right|_{z=L}-\left.\frac{\partial C_1(r,\phi,z,\tau)}{\partial z}\right|_{z=-L}\right]d\phi drdt\int_0^{\Theta}(\Theta-$$
$$t)\int_0^{2\pi}\int_{-L}^{L}\{r[\alpha_{2C}-\alpha_{1C}+C_1(R,\phi,z,\tau)]\cdot[v_r(R,\phi,z,\tau)-\bar{v}_r(R,\phi,z,\tau)]\}dzd\phi dt\times\frac{1}{\pi\Theta R^2L}-$$
$$\frac{V_0}{\pi\Theta R^2L}\int_0^{\Theta}(\Theta-t)\int_0^{R}r\int_0^{2\pi}(\alpha_{2C}-\alpha_{1C}+C_0)dzd\phi drdt.$$

After growing 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 mismatch-induced stress. In this situation to describe the mixing of layers, we use the second Fick's law in the following form [22], [23].

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

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 the 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 the 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 depend on properties of materials of the 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].

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

Here $D_L(x,y,z,T)$ and $D_{LS}(x,y,z,T)$ are the spatial (due to accounting for 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 an integer in the following interval $\gamma \in$[1], [4], [23]. The concentration dependence of diffusion coefficients was described in detail in [23]. Chemical potential μ in (19) could be determined 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 (21) could be transformed into the following form.

$$\mu_1(x,y,z,t)=E(z)\frac{\Omega}{2}\left[\frac{\partial u_i(x,y,z,t)}{\partial x_j}+\frac{\partial u_j(x,y,z,t)}{\partial x_i}\right]\Bigg\{\frac{1}{2}\left[\frac{\partial u_i(x,y,z,t)}{\partial x_j}+\frac{\partial u_j(x,y,z,t)}{\partial x_i}\right]-\varepsilon_0\delta_{ij}+$$
$$\frac{\sigma(z)\delta_{ij}}{1-2\sigma(z)}\Bigg[\frac{\partial u_k(x,y,z,t)}{\partial x_k}-3\varepsilon_0\Bigg]-K(z)\beta(z)[T(x,y,z,t)-T_0]\delta_{ij}\Bigg\},$$

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

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 coincides (for our case) with room temperature. Components of displacement vector could be obtained by solution of the following [24].

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

Where

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

$\rho(z)$ is the density of materials of the heterostructure, δ_{ij} Is the Kronecker symbol. With account the relation for σ_{ij} last system of the equation could be written as (22).

$$\rho(z)\frac{\partial^2 u_x(x,y,z,t)}{\partial t^2}=\left\{K(z)+\frac{5E(z)}{6[1+\sigma(z)]}\right\}\frac{\partial^2 u_x(x,y,z,t)}{\partial x^2}+\left\{K(z)-\frac{E(z)}{3[1+\sigma(z)]}\right\}\times\frac{\partial^2 u_y(x,y,z,t)}{\partial x\partial y}+$$
$$\frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial^2 u_y(x,y,z,t)}{\partial y^2}+\frac{\partial^2 u_z(x,y,z,t)}{\partial z^2}\right]+\left[K(z)+\frac{E(z)}{3[1+\sigma(z)]}\right]\times\frac{\partial^2 u_z(x,y,z,t)}{\partial x\partial z}-K(z)\beta(z)\frac{\partial T(x,y,z,t)}{\partial x}$$
$$\rho(z)\frac{\partial^2 u_y(x,y,z,t)}{\partial t^2}=\frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial^2 u_y(x,y,z,t)}{\partial x^2}+\frac{\partial^2 u_x(x,y,z,t)}{\partial x\partial y}\right]-\frac{\partial T(x,y,z,t)}{\partial y}\times K(z)\beta(z)+$$
$$\frac{\partial}{\partial z}\left\{\frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial u_y(x,y,z,t)}{\partial z}+\frac{\partial u_z(x,y,z,t)}{\partial y}\right]\right\}+\frac{\partial^2 u_y(x,y,z,t)}{\partial y^2}$$
$$\times\left\{\frac{5E(z)}{12[1+\sigma(z)]}+K(z)\right\}+\left\{K(z)-\frac{E(z)}{6[1+\sigma(z)]}\right\}\frac{\partial^2 u_y(x,y,z,t)}{\partial y\partial z}+K(z)\frac{\partial^2 u_y(x,y,z,t)}{\partial x\partial y}$$
$$\rho(z)\frac{\partial^2 u_z(x,y,z,t)}{\partial t^2}=\frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial^2 u_z(x,y,z,t)}{\partial x^2}+\frac{\partial^2 u_z(x,y,z,t)}{\partial y^2}+\frac{\partial^2 u_x(x,y,z,t)}{\partial x\partial z}+\frac{\partial^2 u_y(x,y,z,t)}{\partial y\partial z}\right]+$$
$$\frac{\partial}{\partial z}\left\{K(z)\left[\frac{\partial u_x(x,y,z,t)}{\partial x}+\frac{\partial u_y(x,y,z,t)}{\partial y}+\frac{\partial u_x(x,y,z,t)}{\partial z}\right]\right\}+\frac{1}{6}\frac{\partial}{\partial z}\Bigg\{\frac{E(z)}{1+\sigma(z)}\Bigg[6\frac{\partial u_z(x,y,z,t)}{\partial z}-\frac{\partial u_x(x,y,z,t)}{\partial x}-$$
$$\frac{\partial u_y(x,y,z,t)}{\partial y}-\frac{\partial u_z(x,y,z,t)}{\partial z}\Bigg]\Bigg\}-K(z)\beta(z)\frac{\partial T(x,y,z,t)}{\partial z} \qquad (22)$$

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

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

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

$$\rho_1(x,y,z,t)=\alpha_{1C}\Omega\frac{\partial}{\partial x}\int_0^t D_{SL}(x,y,z,T)\nabla_S\mu_1(x,y,z,\tau)\frac{z}{kT}\left[1+\frac{\xi_S\alpha_{1C}^{\gamma}}{P^{\gamma}(x,y,z,T)}\right]d\tau+$$
$$\alpha_{1C}\Omega\frac{\partial}{\partial y}\int_0^t D_{SL}(x,y,z,T)\nabla_S\mu_1(x,y,z,\tau)\frac{z}{kT}\left[1+\frac{\xi_S\alpha_{1C}^{\gamma}}{P^{\gamma}(x,y,z,T)}\right]d\tau+f_\rho(x,y,z) \quad (19a)$$

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

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

Substitution of relation (19*a*) into relation (23) allows obtaining the desired average values in the following form: $\alpha_{1\rho}=\frac{1}{L_xL_yL_z}\int_0^{L_x}\int_0^{L_y}\int_0^{L_z}f_\rho(x,y,z)dzdydx$. 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 [16]. The required approximation was calculated by the following relation.

$$\rho_2(x,y,z,t)=\frac{\partial}{\partial z}\int_0^t D_L(x,y,z,T)\frac{\partial\rho_1(x,y,z,\tau)}{\partial z}\left\{1+\xi\frac{[\alpha_{2C}+\rho_1(x,y,z,\tau)]^{\gamma}}{P^{\gamma}(x,y,z,T)}\right\}d\tau+f_\rho(x,y,z)+$$
$$\Omega\frac{\partial}{\partial x}\int_0^t\frac{D_S}{kT}\nabla_S\mu(x,y,z,\tau)\int_0^{L_z}\left[\alpha_{2\rho}+\rho_1(x,y,W,\tau)\right]dW\,d\tau+\Omega\frac{\partial}{\partial y}\int_0^t\frac{D_S}{kT}\nabla_S\mu(x,y,z,\tau)\int_0^{L_z}\left[\alpha_{2\rho}+\right.$$
$$\left.\rho_1(x,y,W,\tau)\right]dW\,d\tau. \quad (19b)$$

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

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

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

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

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

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

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

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

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:

$$
\begin{aligned}
&\rho(z)\frac{\partial^2 u_{2x}(x,y,z,t)}{\partial t^2}=\Bigl\{K(z)+\frac{5E(z)}{6[1+\sigma(z)]}\Bigr\}\frac{\partial^2 u_{1x}(x,y,z,t)}{\partial x^2}+\Bigl\{K(z)-\frac{E(z)}{3[1+\sigma(z)]}\Bigr\}\frac{\partial^2 u_{1y}(x,y,z,t)}{\partial x\partial y}+\\
&\times\frac{\partial^2 u_{1y}(x,y,z,t)}{\partial x\partial y}+\frac{E(z)}{2[1+\sigma(z)]}\Bigl[\frac{\partial^2 u_{1y}(x,y,z,t)}{\partial y^2}+\frac{\partial^2 u_{1z}(x,y,z,t)}{\partial z^2}\Bigr]-\frac{\partial T(x,y,z,t)}{\partial x}\times\\
&\times K(z)\beta(z)+\Bigl\{K(z)+\frac{E(z)}{3[1+\sigma(z)]}\Bigr\}\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)]}\Bigl[\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}\Bigr]-\frac{\partial T(x,y,z,t)}{\partial y}\times\\
&\times K(z)\beta(z)+\frac{\partial}{\partial z}\Bigl\{\frac{E(z)}{2[1+\sigma(z)]}\Bigl[\frac{\partial u_{1y}(x,y,z,t)}{\partial z}+\frac{\partial u_{1z}(x,y,z,t)}{\partial y}\Bigr]\Bigr\}+\frac{\partial^2 u_{1y}(x,y,z,t)}{\partial y^2}\times\\
&\times\Bigl\{\frac{5E(z)}{12[1+\sigma(z)]}+K(z)\Bigr\}+\Bigl\{K(z)-\frac{E(z)}{6[1+\sigma(z)]}\Bigr\}\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)]}\Bigl[\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}+\\
&+\frac{\partial^2 u_{1y}(x,y,z,t)}{\partial y\partial z}\Bigr]+\frac{\partial}{\partial z}\Bigl\{K(z)\Bigl[\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}\Bigr]\Bigr\}+\\
&+\frac{E(z)}{6[1+\sigma(z)]}\frac{\partial}{\partial z}\Bigl[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}\Bigr]-\\
&-\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}\Bigr]\Bigr\}\frac{E(z)}{1+\sigma(z)}-K(z)\beta(z)\frac{\partial T(x,y,z,t)}{\partial z}.
\end{aligned}
$$

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

$$
\begin{aligned}
&u_{2x}(x,y,z,t)=\frac{1}{\rho(z)}\Bigl\{K(z)+\frac{5E(z)}{6[1+\sigma(z)]}\Bigr\}\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)}\Bigl\{K(z)-\\
&-\frac{E(z)}{3[1+\sigma(z)]}\Bigr\}\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)}\Bigl[\frac{\partial^2}{\partial y^2}\int_0^t\int_0^{\vartheta}u_{1y}(x,y,z,\tau)d\tau d\vartheta+\\
&+\frac{\partial^2}{\partial z^2}\int_0^t\int_0^{\vartheta}u_{1z}(x,y,z,\tau)d\tau d\vartheta\Bigr]\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\,\Bigl\{K(z)+\\
&+\frac{E(z)}{3[1+\sigma(z)]}\Bigr\}-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)}\Bigl\{K(z)+\frac{5E(z)}{6[1+\sigma(z)]}\Bigr\}-\Bigl\{K(z)-\frac{E(z)}{3[1+\sigma(z)]}\Bigr\}\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)]}\Bigl[\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\Bigr]-\\
&-\frac{1}{\rho(z)}\Bigl\{K(z)+\frac{E(z)}{3[1+\sigma(z)]}\Bigr\}\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)[1+\sigma(z)]}\Bigl[\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\Bigr]+\\
&\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)}\Bigl\{\frac{5E(z)}{12[1+\sigma(z)]}+K(z)\Bigr\}\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}\Bigl\{\frac{E(z)}{1+\sigma(z)}\Bigl[\frac{\partial}{\partial z}\int_0^t\int_0^{\vartheta}u_{1y}(x,y,z,\tau)d\tau d\vartheta+\\
&+\frac{\partial}{\partial y}\int_0^t\int_0^{\vartheta}u_{1z}(x,y,z,\tau)d\tau d\vartheta\Bigr]\Bigr\}-K(z)\frac{\beta(z)}{\rho(z)}\int_0^t\int_0^{\vartheta}T(x,y,z,\tau)d\tau d\vartheta-\Bigl\{\frac{E(z)}{6[1+\sigma(z)]}-\\
&-K(z)\Bigr\}\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)}\Bigl[\frac{\partial^2}{\partial x^2}\int_0^{\infty}\int_0^{\vartheta}u_{1x}(x,y,z,\tau)d\tau d\vartheta+\\
&+\frac{\partial^2}{\partial x\partial y}\int_0^{\infty}\int_0^{\vartheta}u_{1x}(x,y,z,\tau)d\tau d\vartheta\Bigr]\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\,\Bigl\{\frac{5E(z)}{12[1+\sigma(z)]}+\\
&+K(z)\Bigr\}-\frac{\partial}{\partial z}\Bigl\{\frac{E(z)}{1+\sigma(z)}\Bigl[\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\Bigr]\Bigr\}\times\\
&\times\frac{1}{2\rho(z)}-\frac{1}{\rho(z)}\Bigl\{K(z)-\frac{E(z)}{6[1+\sigma(z)]}\Bigr\}\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)]}\Bigl[\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+\\
&+\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\Bigr]\frac{1}{\rho(z)}+\frac{1}{\rho(z)}\times\\
&\times\frac{\partial}{\partial z}\Bigl\{K(z)\Bigl[\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+\\
&+\frac{\partial}{\partial z}\int_0^{\infty}\int_0^{\vartheta}u_{1x}(x,y,z,\tau)d\tau d\vartheta\Bigr]\Bigr\}+\frac{1}{6\rho(z)}\frac{\partial}{\partial z}\Bigl\{\frac{E(z)}{1+\sigma(z)}\Bigl[6\frac{\partial}{\partial z}\int_0^{\infty}\int_0^{\vartheta}u_{1z}(x,y,z,\tau)d\tau d\vartheta-
\end{aligned}
$$

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

In this paper, we calculate concentrations of a mixture of gases and a diffusing material in the considered heterostructure, distribution of temperature, and components of displacement vector as the second-order approximations in the framework of 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 comparing them with the results of numerical simulation.

3. DISCUSSION

In this section, we analyzed the diffusion mixing of the heterostructure layers during annealing with account for the relaxation of mismatch-induced stresses. Typical distributions of diffusant concentrations in the considered heterostructure are shown in Figure 2 for the 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 as shown in Figure 3. It should be noted that the porosity of the buffer layer leads to increasing this effect.

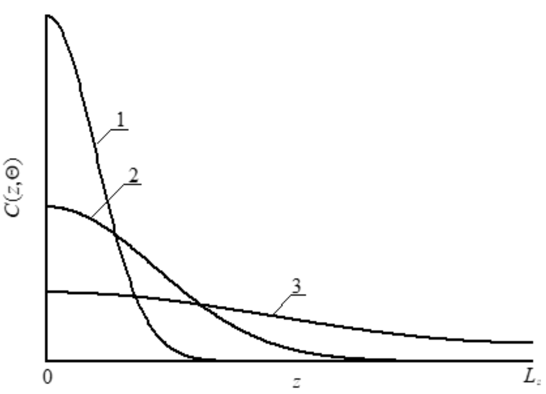

Figure 2. Spatial distributions of diffusant in the considered heterostructure at different values of the continuance of annealing time. Increasing of number of curves corresponds to increasing the continuance of annealing time

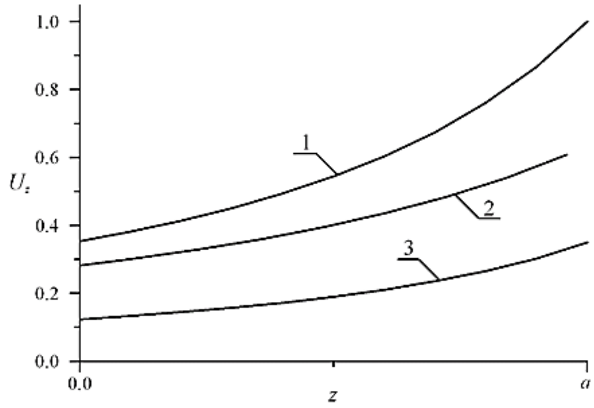

Figure 3. Normalized dependences of the component of the displacement vector u_z on the z coordinate (a is the thickness of the buffer layer). Increasing of number of curves corresponds to increasing the continuance of annealing time

4. CONCLUSION

In this paper, we analyzed the effect of processing the substrate, which precedes the growth of new epitaxial layers, on the 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 decreases the value of mismatch-induced stresses. An analytical approach has been introduced for the analysis of mass and heat transfer in a multilayer structure with account mismatch-induced stress.

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