COMPUTER
METHODS
IN MATERIALS
SCIENCE

2022, vol. 22, no. 2, 89–100
https://doi.org/10.7494/cmms.2022.2.0790

On changing the properties of a multilayer structure by preliminary processing of a substrate

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Abstract

In this paper, the effect of the preliminary processing of a substrate on the properties of a grown heterostructure is investigated. It is shown that the growth of an epitaxial layer on a buffer layer after preliminary annealing (before the growth) 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 accounting for mismatch-induced stress.

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

1. Introduction

In the manufacture of various devices with solid-state electronics, heterostructures of different configurations are frequently used. For their growth, different methods can be employed: gas phase and liquid phase epitaxy, sputtering of materials in magnetrons, and molecular beam epitaxy. The manufacturing technologies and further use of heterostructures in different devices have already been described in a large number of experimental works (Bravo-García et al., 2015; Chakraborty et al., 2004; Gusev & Gusev, 1991; Lachin & Savelov, 2001; Li et al. 2006; Lundin et al., 2009; Mitsuhara, 1998; Stepanenko, 1980; Sorokin et al., 2008; Taguchi et al., 2016; Vorob'ev et al., 2003). At the same time, fewer works have described the prediction of epitaxy processes (Kukushkin et al., 2001; Talalaev et al., 2001). Therefore, 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 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 was placed together with a gas carrier 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 resulting structure was annealed. After that, an epitaxial layer was grown. The main aim of the present paper is to analyze of changes in the properties of the heterostructure accounting for the role of annealing. An accompanying aim of this paper is the introduction of an analytical approach for the analysis of mass and heat transfer in multilayer structures considering their

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nonlinearity, changes of processes parameters in space and time, as well as mismatch-induced stresses.

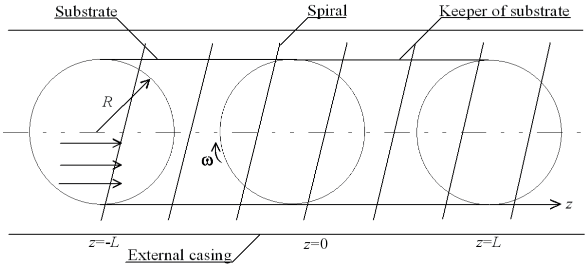

Fig. 1. A reactor for the gas phase epitaxy in the area of the reaction zone

2. Method of solution

The aim of the present paper will be achieved by analyzing the spatio-temporal distribution of temperature and the concentration of the deposited material. We calculate spatio-temporal distribution of temperature during the growth of the epitaxial layer and annealing of heterostructure by solution of the second Fourier law in the following form (Carslaw & Jaeger, 1964):

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

where vector $\vec{v}$ is the speed of flow of the considered mixture of gases; parameter c is the capacity of heat; function $T(r, \varphi, z, t)$ is the distribution of temperature in space and time; function $p(r, \varphi, z, t)$ describes the power density, which standing out in the considered system substrate – keeper of substrate by induction heating by using alternative current in spiral around keeper of substrate and substrate; 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 can be determined by the following 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 is 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. The last term of Equation (1) describes convection during the growth of films. This term will be equal to zero during the annealing of the heterostructure without the growth of new layers.

To solve the above equation, one should take into account the movement of the mixture of gases and the concentration of this mixture. Therefore, we calculate the required values by solving the equation of Navier–Stokes (see Eq. (2)) and Fick's second law with the convective term (i.e. with the second term in the right side of the law (see Eq. (3)). We consider that radius of the keeper of substrate R is significantly larger than the thickness of diffusion and near-boundary layers. We also assume that the stream of gas is laminar. In this situation, the appropriate equations can be written as:

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

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

where D is the diffusion coefficient of a mixture of gases (gases-reagents and gas-carrier); P is the pressure; ν is the kinematics 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:

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

Here parameter σ is equal to σ = 5,67 × 10^{-8} $W \times m^{-2} \times K^{-4}$, parameter T_r describes the room temperature, parameter ω describes the frequency of rotation of the substrate. Zero and periodic boundary conditions correspond to the absence of flow through appropriate interfaces. Non-zero boundary conditions correspond to the reception of materials into the reaction chamber.

Equations for components of the velocity of flow in the cylindrical system of coordinate can be written as:

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

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

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

We determine the solution of this system of equations by using the method of averaging of function corrections (Pankratov, 2012; Pankratov & Bulaeva, 2012, 2013a, 2013b, 2013c, 2013d, 2015; Sokolov, 1955). In the framework of this approach, one should determine the first-order approximation of components of the speed of flow of a mixture of gases and replace the required functions on their average values $v_r \to a_{1r}$, $v_\text{j} \to a_{1\text{j}}$, $v_z \to a_{1z}$ on the right sides of the Equations of the system (5). After the replacement, we obtain equations for the first-order approximations of the components:

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

The solutions to the above equations are:

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

The second-order approximations of components of velocity of flow were obtained by replacement of the required functions on the following sums $v_r \to \alpha_{1r}$, $v_\varphi \to \alpha_{1\varphi}$, $v_z \to \alpha_{1z}$. Equations for the considered approximations take the form:

$$\frac{\partial v_{2r}}{\partial t} = \nu\left(\frac{\partial^2 v_{1r}}{\partial r^2} + \frac{\partial^2 v_{1r}}{\partial r \partial z} - \frac{\partial^2 v_{1r}}{\partial z^2} + \frac{\partial^2 v_{1z}}{\partial r \partial z}\right) - \frac{\partial}{\partial r}\left(\frac{P}{\xi}\right) - (\alpha_{2r} + v_{1r})\frac{\partial v_{1r}}{\partial r} - \frac{(\alpha_{2\varphi} + v_{1\varphi})}{r}\frac{\partial v_{1r}}{\partial \varphi} - (\alpha_{2z} + v_{1z})\frac{\partial v_{1r}}{\partial z} \tag{8a}$$

$$\frac{\partial v_{2\varphi}}{\partial t} = \nu\left(\frac{1}{r}\frac{\partial^2 v_{1r}}{\partial r \partial \varphi} + \frac{2}{r^2}\frac{\partial^2 v_{1\varphi}}{\partial \varphi^2} - \frac{1}{r^2}\frac{\partial^2 v_{1r}}{\partial \varphi \partial z} + \frac{\partial^2 v_{1\varphi}}{\partial z^2}\right) - (\alpha_{2r} + v_{1r})\frac{\partial v_{1\varphi}}{\partial r} - \frac{(\alpha_{2\varphi} + v_{1\varphi})}{r}\frac{\partial v_{1\varphi}}{\partial \varphi} - (\alpha_{2z} + v_{1z})\frac{\partial v_{1\varphi}}{\partial z} - \frac{1}{r}\frac{\partial}{\partial \varphi}\left(\frac{P}{\xi}\right) \tag{8b}$$

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

Integration of the above equations leads to the following result:

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

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

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

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

$$\begin{gathered}
\alpha_{2r} = \frac{1}{\pi \Theta R^2 L} \int\limits_0^\Theta \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^{L} \left(v_{2r} - v_{1r}\right) d\,z\,d\,\varphi\,d\,r\,d\,t \\
\alpha_{2\varphi} = \frac{1}{\pi \Theta R^2 L} \int\limits_0^\Theta \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^{L} \left(v_{2\varphi} - v_{1\varphi}\right) d\,z\,d\,\varphi\,d\,r\,d\,t \qquad (9) \\
\alpha_{2z} = \frac{1}{\pi \Theta R^2 L} \int\limits_0^\Theta \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^{L} \left(v_{2z} - v_{1z}\right) d\,z\,d\,\varphi\,d\,r\,d\,t
\end{gathered}$$

where Θ is the duration of the moving of the mixture of gases through the reactor. The substitution of the first- and the second-order approximations of the required components of velocity into the relation (9) provides us with the opportunity to obtain a system of equations to determine the required average values:

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

where:

$$A_1 = 1 + \int\limits_0^\Theta (\Theta - t) \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^{L} \frac{\partial v_{1r}}{\partial r} d\,z\,d\,\varphi\,d\,r\,d\,t$$

$$C_1 = C_2 = \frac{\pi}{2} \Theta^2 R^2 V_0$$

$$B_1 = \int\limits_0^\Theta (\Theta - t) \int\limits_0^R \int\limits_0^{2\pi} \int\limits_{-L}^{L} \frac{\partial v_{1r}}{\partial \varphi} d\,z\,d\,\varphi\,d\,r\,d\,t$$

$$\begin{gathered}
D_1 = \nu \int\limits_0^\Theta \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^{L} \left(\frac{\partial^2 v_{1r}}{\partial r^2} + \frac{\partial^2 v_{1r}}{\partial r \partial z} - \frac{\partial^2 v_{1r}}{\partial z^2} + \frac{\partial^2 v_{1z}}{\partial r \partial z} \right) dz \times \\
d\varphi\, dr \left(\Theta - t\right) dt - \frac{\pi}{8} \Theta^2 R^2 V_0^2 - \int\limits_0^\Theta (\Theta - t) \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^{L} v_{1r} \times \\
\frac{\partial v_{1r}}{\partial r} dz\, d\varphi\, dr\, dt - \int\limits_0^\Theta (\Theta - t) \int\limits_0^R \int\limits_0^{2\pi} \int\limits_{-L}^{L} v_{1\varphi} \frac{\partial v_{1r}}{\partial \varphi} dz\, d\varphi\, dr\, dt
\end{gathered}$$

$$B_2 = 1 + \int\limits_0^\Theta (\Theta - t) \times \int\limits_0^R \int\limits_0^{2\pi} \int\limits_{-L}^{L} \frac{\partial v_{1r}}{\partial \varphi} dz\, d\varphi\, dr\, dt$$

$$A_2 = \int\limits_0^\Theta \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^{L} \frac{\partial v_{1r}}{\partial r} d\,z\,d\,\varphi\,d\,r \times \left(\Theta - t\right) dt$$

$$\begin{gathered}
D_2 = \nu \int\limits_0^\Theta (\Theta - t) \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^{L} \left(\frac{1}{r} \frac{\partial^2 v_{1r}}{\partial r \partial \varphi} + \frac{2}{r^2} \frac{\partial^2 v_{1\varphi}}{\partial \varphi^2} - \right. \\
\left. \frac{1}{r^2} \frac{\partial^2 v_{1r}}{\partial \varphi \partial z} + \frac{\partial^2 v_{1\varphi}}{\partial z^2} \right) d\,z\,d\,\varphi\,d\,r\,d\,t - \frac{\pi}{8} \Theta^2 R^2 V_0^2 - \\
\int\limits_0^\Theta (\Theta - t) \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^{L} v_{1r} \frac{\partial v_{1r}}{\partial r} d\,z\,d\,\varphi\,d\,r\,d\,t - \\
\int\limits_0^\Theta (\Theta - t) \int\limits_0^R \int\limits_0^{2\pi} \int\limits_{-L}^{L} v_{1\varphi} \frac{\partial v_{1r}}{\partial \varphi} d\,z\,d\,\varphi\,d\,r\,d\,t
\end{gathered}$$

$$A_3 = \int\limits_0^\Theta (\Theta - t) \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^{L} \frac{\partial v_{1z}}{\partial r} d\,z\,d\,\varphi\,d\,r\,d\,t$$

$$B_3 = \int\limits_0^\Theta (\Theta - t) \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^{L} \frac{\partial v_{1z}}{\partial \varphi} d\,z\,d\,\varphi\,d\,r\,d\,t$$

$$C_3 = 1 + \frac{\pi}{2} \Theta^2 V_0 \times R^2$$

$$\begin{gathered}
D_3 = \nu \int\limits_0^\Theta \int\limits_0^R \int\limits_0^{2\pi} \int\limits_{-L}^{L} \left(\frac{\partial^2 v_{1r}}{\partial z^2} + \frac{\partial^2 v_{1z}}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2 v_{1z}}{\partial \varphi^2} \right) d\,z\,d\,\varphi \times \\
r\,d\,r\,\left(\Theta - t\right) d\,t - \int\limits_0^\Theta (\Theta - t) \int\limits_0^R r\,d\,r \left(\Theta - t\right) d\,t - \\
\int\limits_0^\Theta (\Theta - t) \int\limits_0^R r \int\limits_0^{2\pi} \int\limits_{-L}^{L} v_{1\varphi} \frac{\partial v_{1z}}{\partial \varphi} d\,z\,d\,\varphi\,d\,r\,d\,t - \frac{\pi}{8} \Theta^2 R^2 V_0^2
\end{gathered}$$

The solution of the above system of equations was calculated by standard approaches (Korn & Korn, 1968) and can be written as:

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

where:

$$\begin{gathered}
\Delta = A_1 \left(B_2 C_3 - B_3 C_2\right) - B_1 \left(A_2 C_3 - A_3 C_2\right) + C_1 \left(A_2 B_3 - A_3 B_2\right) \\
\Delta_r = D_1 \left(B_2 C_3 - B_3 C_2\right) - B_1 \left(D_2 C_3 - D_3 C_2\right) + C_1 \left(D_2 B_3 - D_3 B_2\right) \\
\Delta_\varphi = D_1 \left(B_2 C_3 - B_3 C_2\right) - B_1 \left(D_2 C_3 - D_3 C_2\right) + C_1 \left(D_2 B_3 - D_3 B_2\right) \\
\Delta_z = A_1 \left(B_2 D_3 - B_3 D_2\right) - B_1 \left(A_2 D_3 - A_3 D_2\right) + D_1 \left(A_2 B_3 - A_3 B_2\right)
\end{gathered}$$

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

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

$$\begin{gathered}\frac{1}{r}\frac{\partial}{\partial r}\left[r\,D\frac{\partial C(r,\varphi,z,t)}{\partial r}\right]+\frac{\partial}{\partial z}\left[D\frac{\partial C(r,\varphi,z,t)}{\partial z}\right]-\\ \frac{1}{r}\frac{\partial}{\partial r}\left\{r\,C(r,\varphi,z,t)\cdot\left[v_r(r,\varphi,z,t)-\bar{v}_r(r,\varphi,z,t)\right]\right\}-\\ \frac{1}{r}\frac{\partial}{\partial \varphi}\left\{r\,C(r,\varphi,z,t)\cdot\left[v_\phi(r,\varphi,z,t)-\bar{v}_\phi(r,\varphi,z,t)\right]\right\}-\\ \frac{\partial}{\partial z}\left\{C(r,\varphi,z,t)\cdot\left[v_z(r,\varphi,z,t)-\bar{v}_z(r,\varphi,z,t)\right]\right\}\end{gathered}\tag{13}$$

We calculate the distribution of temperature in space and time and the same distribution of concentration of a mixture of gases. Once again, we can use the method of an average of function corrections. To calculate the first-order approximations of the required functions, we replace their not yet known average values α_{1T} and α_{1C} in the right sides of the above equations. Further, we can use a recently considered algorithm to obtain the first-order approximations of the temperature and concentration of a gas mixture:

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

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

The above not yet known average values were calculated by the standard relations:

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

The substitution of the first-order approximations of temperature and concentration of a gas mixture into relations (16) gives us the following results:

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

$$\begin{gathered}\alpha_{1T}=\left[T_r+\int_0^\Theta\frac{(\Theta-t)}{\pi\Theta R^2L}\int_0^R r\int_0^{2\pi}\int_{-L}^{L}\frac{p(r,\varphi,z,t)}{c}d z\,d\varphi\,d r\,d t\right]\times\\ \left(1+\frac{C_0}{\pi\Theta RL^2}\left\{\int_0^\Theta(\Theta-t)\int_0^{2\pi}\int_{-L}^{L}\left[v_r(R,\varphi,z,\tau)-\right.\right.\right.\\ \left.\bar{v}_r(R,\varphi,z,\tau)\right]d z\,d\varphi\,d t+\frac{V_0}{2}-\frac{1}{\pi\Theta R^2}\int_0^\Theta(\Theta-t)\times\\ \left.\int_0^R\int_0^{2\pi}\int_{-L}^{L}\left[v_r(r,\varphi,z,t)-\bar{v}_r(r,\varphi,z,t)\right]d z\,d\varphi\,d r\right\}\times\\ \left\{\frac{1}{\pi\Theta R\,L}\times\int_0^\Theta(\Theta-t)\int_0^{2\pi}\int_{-L}^{L}\left[v_r(R,\varphi,z,\tau)-\right.\right.\\ \left.\left.\left.\bar{v}_r(R,\varphi,z,\tau)d z\,d\varphi\,d t+1+\frac{\Theta V_0}{R\,L}\right\}^{-1}\right)\end{gathered}$$

The second-order approximations of temperature and concentration of a mixture of gases we determine in the framework of the method of averaging of function corrections (Pankratov, 2012; Pankratov & Bulaeva, 2012, 2013a, 2013b, 2013c; Sokolov, 1955), i.e. by replacement of the required functions in right sides of Equations (12) and (13) on the following sums $T \rightarrow a_{2T} + T_1$, $C \rightarrow a_{2C} + C_1$. In this case, the second-order approximations of the above required functions can be written as:

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

$$\begin{gathered}C_2(r,\varphi,z,t)=\frac{1}{r^2}\frac{\partial}{\partial\varphi}\int_0^t D\frac{\partial C_1(r,\varphi,z,\tau)}{\partial\varphi}d\tau+\\ C_0\delta(z+L)+\frac{1}{r}\frac{\partial}{\partial r}\int_0^t r\,D\frac{\partial C_1(r,\varphi,z,\tau)}{\partial r}d\tau+\\ \frac{\partial}{\partial z}\int_0^t D\frac{\partial C_1(r,\varphi,z,\tau)}{\partial z}d\tau-\frac{1}{r}\times\\ \frac{\partial}{\partial r}\left\{r\int_0^t\left[\alpha_{2C}+C_1(r,\varphi,z,\tau)\right]\cdot\left[v_r(r,\varphi,z,\tau)-\bar{v}_r(r,\varphi,z,\tau)\right]d\tau\right\}-\end{gathered}\tag{18}$$

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

Average 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:

$$\alpha_{2T}=\frac{1}{\pi\Theta R^2L}\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^{L}\left(T_2-T_1\right)dz\,d\varphi\,dr\,dt$$
$$\alpha_{2C}=\frac{1}{\pi\Theta R^2L}\int_0^\Theta\int_0^R r\int_0^{2\pi}\int_{-L}^{L}\left(C_2-C_1\right)dz\,d\varphi\,dr\,dt \tag{19}$$

The substitution of the first- and the second-order approximations of temperature and concentration of mixture into relations (19) give us the possibility to obtain equations to determine required average values:

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

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

After growing the buffer layer, we consider annealing of 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 Fick's second law in the following form (Gotra, 1991; Zhang & Bower, 1999):

$$\frac{\partial\rho\left(x,y,z,t\right)}{\partial t}=\Omega\frac{\partial}{\partial x}\left[\frac{D_S}{kT}\nabla_S\mu\left(x,y,z,t\right)\times\right.$$
$$\left.\int_0^{L_z}\rho\left(x,y,W,t\right)dW\right]+\Omega\frac{\partial}{\partial y}\left[\frac{D_S}{kT}\nabla_S\mu\left(x,y,z,t\right)\times\right. \tag{20}$$
$$\left.\int_0^{L_z}\rho\left(x,y,W,t\right)dW\right]+\frac{\partial}{\partial z}\left[D\frac{\partial\rho\left(x,y,z,t\right)}{\partial z}\right]$$

with initial and boundary conditions defined as:

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

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; $\int_0^{L_z}\rho\left(x,y,z,t\right)dz$ 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 diffusion coefficients depend on the 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 diffusion coefficients on parameters could be approximated by the following relations (Gotra, 1991):

$$\begin{aligned} D_C &= D_L\left(x,y,z,T\right)\left[1+\xi\frac{\rho^{\gamma}\left(x,y,z,t\right)}{P^{\gamma}\left(x,y,z,T\right)}\right] \\ D_S &= D_{SL}\left(x,y,z,T\right)\left[1+\xi_S\frac{\rho^{\gamma}\left(x,y,z,t\right)}{P^{\gamma}\left(x,y,z,T\right)}\right] \end{aligned} \tag{21}$$

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 an integer in the following interval $\gamma \in [1, 3]$ (Gotra, 1991). The concentrational dependence of diffusion coefficients was described in detail in (Gotra, 1991). The chemical potential μ in Equation (20) can be determined by the following relation (Landau & Lifshits, 2001):

$$\mu = \frac{E(z)\Omega\sigma_{ij}[u_{ij}(x,y,z,t)+u_{ji}(x,y,z,t)]}{2} \tag{22}$$

where $E(z)$ is the Young modulus, σ_{ij} is the stress tensor; $u_{ij} = (\partial u_i/\partial x_j + \partial u_j/\partial x_i)/2$ 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. Equation (22) can be transformed into the following form:

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

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. The components of the displacement vector can be obtained by the solution of the following equations (Landau & Lifshits, 2001):

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

where:

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

$\rho(z)$ is the density of materials of the heterostructure; δ_{ij} is the Kronecker symbol. Considering the relation for σ_{ij} the last system of equations could be written as:

$$\rho\left(z\right)\frac{\partial^2 u_x\left(x,y,z,t\right)}{\partial t^2}=\left\{K\left(z\right)+\frac{5E\left(z\right)}{6\left[1+\sigma\left(z\right)\right]}\right\}\times$$
$$\frac{\partial^2 u_x\left(x,y,z,t\right)}{\partial x^2}+\left\{K\left(z\right)-\frac{E\left(z\right)}{3\left[1+\sigma\left(z\right)\right]}\right\}\times$$
$$\frac{\partial^2 u_y\left(x,y,z,t\right)}{\partial x\partial y}+\left[\frac{\partial^2 u_y\left(x,y,z,t\right)}{\partial y^2}+\right. \tag{23}$$
$$\left.\frac{\partial^2 u_z\left(x,y,z,t\right)}{\partial z^2}\right]\frac{E\left(z\right)}{2\left[1+\sigma\left(z\right)\right]}+\left[K\left(z\right)+\frac{E\left(z\right)}{3\left[1+\sigma\left(z\right)\right]}\right]\times$$
$$\frac{\partial^2 u_z\left(x,y,z,t\right)}{\partial x\partial z}-K\left(z\right)\beta\left(z\right)\frac{\partial T\left(x,y,z,t\right)}{\partial x}$$

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

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

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

$$\left.\left.\frac{\partial u_y(x,y,z,t)}{\partial y}-\frac{\partial u_z(x,y,z,t)}{\partial z}\right]\right\}-K(z)\beta(z)\frac{\partial T(x,y,z,t)}{\partial z}$$

Conditions for the system of Equation (8) can 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 diffusing substance's concentration has been calculated using the method of averaging of functional corrections. The first-order approximation can be determined by the following relation:

$$\rho_1(x,y,z,t)=\alpha_{1C}\Omega\frac{\partial}{\partial x}\int_0^t D_{SL}(x,y,z,T)\times$$

$$\nabla_S\mu_1(x,y,z,\tau)\frac{z}{kT}\left[1+\frac{\xi_S\alpha_{1C}^{\gamma}}{P^{\gamma}(x,y,z,T)}\right]d\tau+$$

$$\alpha_{1C}\Omega\frac{\partial}{\partial y}\int_0^t\nabla_S\mu_1(x,y,z,\tau)\frac{z}{kT}\times \tag{20a}$$

$$D_{SL}(x,y,z,T)\left[1+\frac{\xi_S\alpha_{1C}^{\gamma}}{P^{\gamma}(x,y,z,T)}\right]d\tau+f_\rho(x,y,z)$$

The average value of the considered approximation of the considered function can again be calculated by using the standard relation (Pankratov, 2012; Pankratov & Bulaeva, 2012, 2013a, 2013b, 2013c; Sokolov, 1955):

$$\alpha_{1\rho}=\frac{1}{\Theta L_x L_y L_z}\int_0^{\Theta}\int_0^{L_x}\int_0^{L_y}\int_0^{L_z}\rho_1(x,y,z,t)\,dz\,dy\,dx\,dt \tag{24}$$

The substitution of relation (20a) into relation (24) allows the desired average values to be obtained in the following form:

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

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 (Pankratov, 2012; Pankratov & Bulaeva, 2012, 2013a, 2013b, 2013c; Sokolov, 1955). The following relation calculated the required approximation:

$$\rho_2(x,y,z,t)=\frac{\partial}{\partial z}\int_0^t D_L(x,y,z,T)\times$$

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

$$f_\rho(x,y,z)+\Omega\frac{\partial}{\partial x}\int_0^t\frac{D_S}{kT}\nabla_S\mu\,(x,y,z,\tau)\times$$

$$\int_0^{L_z}\left[\alpha_{2\rho}+\rho_1(x,y,W,\tau)\right]dW\,d\tau+\Omega\frac{\partial}{\partial y}\times$$

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

The average value of the second-order approximation of the required concentration $\alpha_{2\rho}$ is also determined using the standard relation (Pankratov, 2012; Pankratov & Bulaeva, 2012, 2013a, 2013b, 2013c; Sokolov, 1955):

$$\alpha_{2\rho}=\int_0^{\Theta}\int_0^{L_x}\int_0^{L_y}\int_0^{L_z}\left[\rho_2(x,y,z,t)-\rho_1(x,y,z,t)\right]dz\,dy\,dx\,dt\times$$

$$\frac{1}{\Theta L_x L_y L_z} \tag{25}$$

The substitution of relations (20a) and (20b) into relation (25) gives a possibility to obtain a relation for the required average value: $\alpha_{2\rho}=0$. Next, let us solve equations of system (23), i.e. to obtain components of the displacement vector. Equations for the first-order approximations of the considered components after appropriate substitution into the Equations (23) takes the form:

$$\begin{cases}\rho(z)\dfrac{\partial^2 u_{1x}(x,y,z,t)}{\partial t^2}=-K(z)\beta(z)\dfrac{\partial T(x,y,z,t)}{\partial x}\\[2ex]\rho(z)\dfrac{\partial^2 u_{1y}(x,y,z,t)}{\partial t^2}=-K(z)\beta(z)\dfrac{\partial T(x,y,z,t)}{\partial y}\\[2ex]\rho(z)\dfrac{\partial^2 u_{1z}(x,y,z,t)}{\partial t^2}=-K(z)\beta(z)\dfrac{\partial T(x,y,z,t)}{\partial z}\end{cases} \tag{23a}$$

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

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

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

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

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

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

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

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

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

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

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

$$\begin{gathered}
u_{2x}(x,y,z,t)=\frac{1}{\rho(z)}\frac{\partial^2}{\partial x^2}\int_0^t\int_0^{\vartheta}u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta\times \\
\Bigl\{K(z)-\frac{5E(z)}{6[1+\sigma(z)]}\Bigr\}+\frac{\partial^2}{\partial x\,\partial y}\int_0^t\int_0^{\vartheta}u_{1y}(x,y,z,\tau)\times \\
d\tau\,d\vartheta\frac{1}{\rho(z)}\Bigl\{K(z)+\frac{E(z)}{3[1+\sigma(z)]}\Bigr\}+ \\
\Bigl[\frac{\partial^2}{\partial y^2}\int_0^t\int_0^{\vartheta}u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{\partial^2}{\partial z^2}\int_0^t\int_0^{\vartheta}u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta\Bigr]\times \\
\frac{E(z)}{2\rho(z)[1+\sigma(z)]}+\frac{1}{\rho(z)}\Bigl\{K(z)+\frac{E(z)}{3[1+\sigma(z)]}\Bigr\}\frac{\partial^2}{\partial x\,\partial z}\times \\
\int_0^t\int_0^{\vartheta}u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta-K(z)\frac{\beta(z)}{\rho(z)}\frac{\partial}{\partial x}\int_0^t\int_0^{\vartheta}T(x,y,z,\tau)\,d\tau\,d\vartheta- \\
\Bigl\{K(z)+\frac{5E(z)}{6[1+\sigma(z)]}\Bigr\}\frac{1}{\rho(z)}\frac{\partial^2}{\partial x^2}\int_0^{\infty}\int_0^{\vartheta}u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta- \\
\Bigl\{K(z)-\frac{E(z)}{3[1+\sigma(z)]}\Bigr\}\frac{1}{\rho(z)}\frac{\partial^2}{\partial x\,\partial y}\int_0^{\infty}\int_0^{\vartheta}u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta- \\
\frac{E(z)}{2\rho(z)[1+\sigma(z)]}\Bigl[\frac{\partial^2}{\partial y^2}\int_0^{\infty}\int_0^{\vartheta}u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta+ \\
\frac{\partial^2}{\partial z^2}\int_0^{\infty}\int_0^{\vartheta}u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta\Bigr]-\frac{1}{\rho(z)}\Bigl\{K(z)+\frac{E(z)}{3[1+\sigma(z)]}\Bigr\}\times \\
\frac{\partial^2}{\partial x\,\partial z}\int_0^{\infty}\int_0^{\vartheta}u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta+u_{0x}+ \\
K(z)\frac{\beta(z)}{\rho(z)}\frac{\partial}{\partial x}\int_0^{\infty}\int_0^{\vartheta}T(x,y,z,\tau)\,d\tau\,d\vartheta
\end{gathered}$$

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

$$\frac{\partial}{\partial y}\int_0^t\int_0^\vartheta u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta\Bigg]\Bigg\}-K(z)\int_0^t\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta\times$$

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

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

$$\frac{\partial^2}{\partial x\,\partial y}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta\Bigg]-\int_0^\infty\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta\times$$

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

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

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

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

$$\frac{\partial^2}{\partial y\,\partial z}\int_0^\infty\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta+u_{0y}$$

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

$$\frac{\partial^2}{\partial y^2}\int_0^\infty\int_0^\vartheta u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{\partial^2}{\partial x\,\partial z}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta+$$

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

$$\Bigg[\frac{\partial}{\partial x}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{\partial}{\partial y}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta+$$

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

$$\Bigg[6\frac{\partial}{\partial z}\int_0^\infty\int_0^\vartheta u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta-\frac{\partial}{\partial x}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta-$$

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

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

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

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 a different continuance of annealing time. The conclusions, in this case, are quite standard: an increase in the duration of annealing leads to a more homogenous distribution of the diffusant. At the same time, the mixing of heterostructure materials leads to decreases in mechanical stresses (see Fig. 3). It should be noted that the porosity of the buffer layer contributes to increasing this effect.

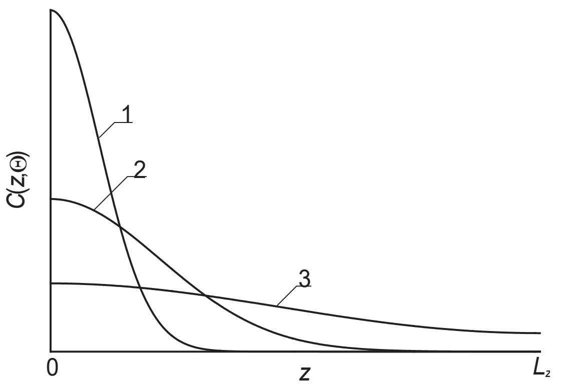

Fig. 2. Spatial distributions of diffusant in the considered heterostructure at different values of a continuance of annealing time. Increasing of number of curves corresponds to increasing the continuance of the annealing time

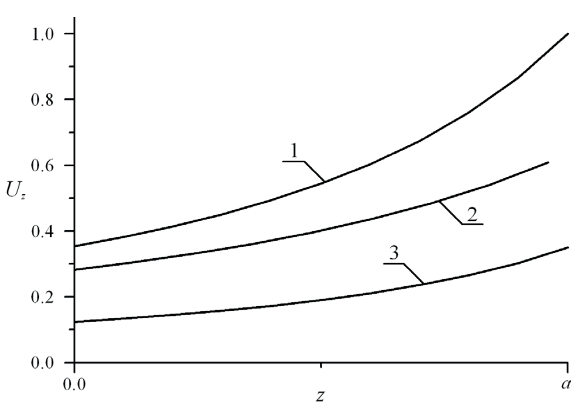

Fig. 3. Normalized dependences of the component of the displacement vector u_z on the z coordinate (a is the thickness of the buffer layer). Increasing of number of curves corresponds to increasing of a continuance of annealing time

4. Conclusion

As presented, we have 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 annealing (before the start of growth) reduces the value of mismatch-induced stresses. An analytical approach has been introduced for the analysis of mass and heat transfer in a multilayer structure considering mismatch-induced stress.

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