VARIATION OF MISMATCH-INDUCED STRESS IN A HETEROSTRUCTURE WITH CHANGING TEMPERATURE OF GROWTH

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ABSTRACT

In this paper we analyzed influence of diffusion of material of an epitaxial layer of a heterostructure during high-temperature growth into next layer (next epitaxial layer or substrate) of the heterostructure on mismatch-induced stress. It has been shown, that value of mismatch-induced stress in heterostructure depends on temperature of growth, because the considered diffusion depends on the temperature. We also introduce an analytical approach to model the diffusion and relaxation of the mismatch-induced stress.

KEYWORDS

Heterostructure; Mismatch-Induced Stress; Temperature Of Growth; Mixing Of Materials Of Layers Of Heterostructure

1. INTRODUCTION

In the present time large number of solid state electronic devices have been manufactured based on heterostructures. The widely using of heterostructures leads to necessity to improve of their properties. It is known, that mismatch-induced stress presents in all heterostructures. The stress in heterostructures could leads to generation misfit dislocations. One way to decrease mismatch-induced stress is choosing materials of heterostructure with as small as possible mismatch of lattice constants [1-3]. Another way to decrease mismatch-induced stress is using a buffer layer, manufactured by using another materials, between layers of heterostructure. Lattice constant of the buffer layer should be average in comparison with lattice constants of nearest layers of heterostructure [4,5].

In this paper we consider a heterostructure with two layers (see Fig. 1). The layers are a substrate and an epitaxial layer. At a high temperature of growth (for example, during epitaxy from gas phase) of heterostructure one can find intensive diffusion of material of the epitaxial layer into the substrate. Our main aim framework the present paper is analysis of variation of mismatch-induced stress in the considered heterostructure with diffusion of material of the epitaxial into the substrate.

2. METHOD OF SOLUTION

Let us to describe diffusion of material of epitaxial layer in the substrate by solution of the following boundary problem [6-11]

$$\frac{\partial\, C(x,y,z,t)}{\partial t}=\frac{\partial}{\partial x}\left[D\frac{\partial C(x,y,z,t)}{\partial x}\right]+\frac{\partial}{\partial y}\left[D\frac{\partial C(x,y,z,t)}{\partial y}\right]+\frac{\partial}{\partial z}\left[D\frac{\partial C(x,y,z,t)}{\partial z}\right]+$$
$$+\Omega\frac{\partial}{\partial x}\left[\frac{D_S}{kT}\nabla_S\mu\,(x,y,z,t)\int_0^{L_z}C(x,y,W,t)\,dW\right]+\Omega\frac{\partial}{\partial y}\left[\frac{D_S}{kT}\nabla_S\mu\,(x,y,z,t)\int_0^{L_z}C(x,y,W,t)\,dW\right] \quad (1)$$

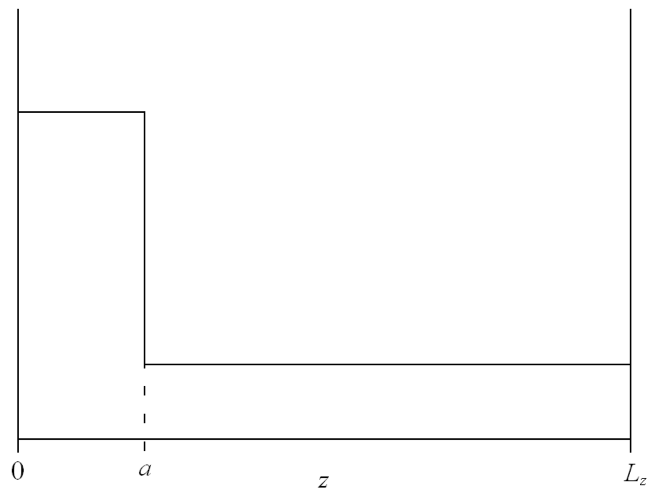

Fig. 1. Heterostructure, which consist of a substrate and an epitaxial layer

$$\left.\frac{\partial C(x,y,z,t)}{\partial x}\right|_{x=L_x}=0,\ \left.\frac{\partial C(x,y,z,t)}{\partial y}\right|_{y=0}=0,\ \left.\frac{\partial C(x,y,z,t)}{\partial y}\right|_{x=L_y}=0,\ \left.\frac{\partial C(x,y,z,t)}{\partial z}\right|_{z=0}=0,$$
$$\left.\frac{\partial C(x,y,z,t)}{\partial z}\right|_{x=L_z}=0,\ C(x,y,z,0)=f_C(x,y,z),\ C(0,y,z,t)=C_0.$$

Here $C(x,y,z,t)$ is the spatio-temporal distribution of concentration of material of epitaxial layer; atomic volume of the dopant describes by Ω; surficial gradient describes by ∇_S; the integral $\int_0^{L_z}C(x,y,z,t)\,dz$ describes surficial concentration of dopant on interface between materials of heterostructure; $\mu(x,y,z,t)$ is the chemical potential; D and D_S are the coefficients of volumetric and surficial diffusions (reason of the surficial diffusion is the mismatch-induced stress). Values of the volumetric and surficial diffusion coefficients are differ in different materials. The diffusion coefficients will be changed in during heating and cooling of heterostructure. Different levels of doping also leads to changing of the diffusion coefficients. We approximate dopant diffusion coefficients by the following functions [7]

$$D_C=D_L(x,y,z,T)\left[1+\xi\frac{C^{\gamma}(x,y,z,t)}{P^{\gamma}(x,y,z,T)}\right],\ D_S=D_{SL}(x,y,z,T)\left[1+\xi_S\frac{C^{\gamma}(x,y,z,t)}{P^{\gamma}(x,y,z,T)}\right]. \quad (2)$$

The functions $D_L(x,y,z,T)$ and $D_{LS}(x,y,z,T)$ describes spatial and temperature dependences of diffusion coefficients. The functions could be obtained by accounting all layers of heterostruicture and Arrhenius law. T is the temperature of grown. $P(x,y,z,T)$ is the limit of solubility of material of the epitaxial layer in the substrate. Parameter γ depends on properties of materials and will be integer in the following interval $\gamma\in[1,3]$ (the dependence described in details in [7]).

Chemical potential μ in the Eq.(1) depends on properties of materials of heterostructure and could be approximated by the following relation [10]

$$\mu=E(z)\Omega\sigma_{ij}\,[u_{ij}(x,y,z,t)+u_{ji}(x,y,z,t)]/2. \qquad (3)$$

Function $E(z)$ describes spatial dependence of Young modulus. Tensor σ_{ij} describes the stress tensor; $u_{ij}=\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)$ is the deformation tensor; u_i, u_j are the components $u_x(x,y,z,t)$, $u_y(x,y,z,t)$ and $u_z(x,y,z,t)$ of the displacement vector $\vec{u}(x,y,z,t)$; x_i, x_j are the coordinate x, y, z. The Eq. (3) could be written in the following equivalent form

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

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

Here σ is Poisson coefficient; the normalized difference $\varepsilon_0=(a_s-a_{EL})/a_{EL}$ describes the mismatch parameter; parameters a_s, a_{EL} in the above difference 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 (in our case) with room temperature. Components of the displacement vector have been described by the following equations [11]

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

The stress tensor σ_{ij} correlates with components of the displacement vector by the following relation $\sigma_{ij}=\frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial u_i(x,y,z,t)}{\partial x_j}+\frac{\partial u_j(x,y,z,t)}{\partial x_i}-\frac{\delta_{ij}}{3}\frac{\partial u_k(x,y,z,t)}{\partial x_k}\right]+\delta_{ij}\frac{\partial u_k(x,y,z,t)}{\partial x_k}\times$ $\times K(z)-\beta(z)K(z)[T(x,y,z,t)-T_r]$.

The function $\rho(z)$ describes the density of materials of heterostructure. The tenzor δ_{ij} describes the Kronecker symbol. Accounting relation for σ_{ij} in the previous system of equations last system of equation could be written as

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

$$\rho(z)\frac{\partial^2 u_y(x,y,z,t)}{\partial t^2}=\frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial^2 u_y(x,y,z,t)}{\partial x^2}+\frac{\partial^2 u_x(x,y,z,t)}{\partial x\partial y}\right]-K(z)\beta(z)\frac{\partial T(x,y,z,t)}{\partial y}+$$
$$+\frac{\partial}{\partial z}\left\{\frac{E(z)}{2[1+\sigma(z)]}\left[\frac{\partial u_y(x,y,z,t)}{\partial z}+\frac{\partial u_z(x,y,z,t)}{\partial y}\right]\right\}+\left\{\frac{5E(z)}{12[1+\sigma(z)]}+K(z)\right\}\frac{\partial^2 u_y(x,y,z,t)}{\partial y^2}+$$
$$+\left\{K(z)-\frac{E(z)}{6[1+\sigma(z)]}\right\}\frac{\partial^2 u_y(x,y,z,t)}{\partial y\partial z}+K(z)\frac{\partial^2 u_y(x,y,z,t)}{\partial x\partial y} \tag{4}$$

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

Conditions for the system of Eqs.(4) are

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

We determine spatio-temporal distributions of concentration of material of epitaxial layer in the substrate by solving the Eq.(1) framework method of averaging of function corrections in the standard form [12,13]. Previously we transform the Eq.(1) to the following form with account initial distributions of the considered concentrations

$$\frac{\partial C(x,y,z,t)}{\partial t}=\frac{\partial}{\partial x}\left[D\frac{\partial C(x,y,z,t)}{\partial x}\right]+\frac{\partial}{\partial y}\left[D\frac{\partial C(x,y,z,t)}{\partial y}\right]+\frac{\partial}{\partial z}\left[D\frac{\partial C(x,y,z,t)}{\partial z}\right]+$$
$$+\Omega\frac{\partial}{\partial x}\left[\frac{D_S}{kT}\nabla_S\mu\,(x,y,z,t)\int_0^{L_z}C(x,y,W,t)\,dW\right]+\Omega\frac{\partial}{\partial y}\left[\frac{D_S}{kT}\nabla_S\mu\,(x,y,z,t)\int_0^{L_z}C(x,y,W,t)\,dW\right]+$$
$$+f_C(x,y,z)\,\delta(t) \tag{1a}$$

After that we replace the required function $C\,(x,y,z,t)$ in right side of Eq. (1*a*) on its not yet known average value α_{1C}. In this situation we obtain equation to determine the first- order approximations of the considered concentrations in the following form

$$\frac{\partial C_1(x,y,z,t)}{\partial t}=\alpha_{1C}\Omega\frac{\partial}{\partial x}\left[z\frac{D_S}{kT}\nabla_S\mu\,(x,y,z,t)\right]+\alpha_{1C}\Omega\frac{\partial}{\partial y}\left[z\frac{D_S}{kT}\nabla_S\mu\,(x,y,z,t)\right]+ + f_C\,(x,y,z)\delta(t). \quad (1b)$$

After integration of the left and right sides of the Eq.(1*b*) gives us possibility to obtain relation for the first-order approximation of concentration of material of the epitaxial layer in the substrate in the following form

$$C_1(x,y,z,t)=\alpha_{1C}\Omega\frac{\partial}{\partial x}\int_0^t D_{SL}(x,y,z,T)\frac{z}{kT}\nabla_S\mu\,(x,y,z,\tau)\left[1+\frac{\xi_S\alpha_{1C}^{\gamma}}{P^{\gamma}(x,y,z,T)}\right]d\tau+ +\alpha_{1C}\frac{\partial}{\partial y}\int_0^t D_{SL}(x,y,z,T)\frac{z}{kT}\nabla_S\mu\,(x,y,z,\tau)\left[1+\frac{\xi_S\alpha_{1C}^{\gamma}}{P^{\gamma}(x,y,z,T)}\right]d\tau+f_C\,(x,y,z) \quad (1c)$$

We determine average values of the first-order approximations of considered concentration by using the following relations [12,13]

$$\alpha_{1C}=\frac{1}{\Theta L_x L_y L_z}\int_0^{\Theta}\int_0^{L_x}\int_0^{L_y}\int_0^{L_z}C_1(x,y,z,t)\,d\,z\,d\,y\,d\,x\,d\,t\,. \quad (5)$$

Substitution of the relation (1*c*) into relation (5) gives us possibility to obtain the following relations

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

Farther we used standard iteration procedure of method of averaging of function corrections [12, 13] to obtain the second-order approximation of concentration of material of epitaxial layer in the substrate. Framework this procedure to calculate *n*-th-order approximation of concentration of material of epitaxial layer in the substrate we replace the required concentration $C(x,y,\,z,t)$ in the right side of Eq. (1*a*) on the following sum $\alpha_{nC}+C_{n-1}(x,y,z,t)$. This substitution gives us possibility to obtain equation for the second-order approximation of the required concentration

$$\frac{\partial C_2(x,y,z,t)}{\partial t}=\frac{\partial}{\partial x}\left(D_L(x,y,z,T)\left\{1+\xi\frac{[\alpha_{2C}+C_1(x,y,z,t)]^{\gamma}}{P^{\gamma}(x,y,z,T)}\right\}\frac{\partial C_1(x,y,z,t)}{\partial x}\right)+ +\frac{\partial}{\partial y}\left(D_L(x,y,z,T)\left\{1+\xi\frac{[\alpha_{2C}+C_1(x,y,z,t)]^{\gamma}}{P^{\gamma}(x,y,z,T)}\right\}\frac{\partial C_1(x,y,z,t)}{\partial y}\right)+\frac{\partial}{\partial z}\left(\frac{\partial C_1(x,y,z,t)}{\partial z}\times \times D_L(x,y,z,T)\left\{1+\xi\frac{[\alpha_{2C}+C_1(x,y,z,t)]^{\gamma}}{P^{\gamma}(x,y,z,T)}\right\}\right)+f_C\,(x,y,z)\delta(t)+\Omega\frac{\partial}{\partial x}\left[\frac{D_S}{kT}\times \times\nabla_S\mu\,(x,y,z,t)\int_0^{L_z}C_1(x,y,W,t)\,dW\right]+\Omega\frac{\partial}{\partial y}\left[\frac{D_S}{kT}\nabla_S\mu\,(x,y,z,t)\int_0^{L_z}C_1(x,y,W,t)\,dW\right]. \quad (1d)$$

After integration of the left and right sides of the Eq.(1*d*) gives us possibility to obtain relation for the second-order approximation of concentration of material of the epitaxial layer in the substrate in the following form

$$C_2(x,y,z,t)=\frac{\partial}{\partial x}\int_0^t D_L(x,y,z,T)\left\{1+\xi\frac{[\alpha_{2C}+C_1(x,y,z,\tau)]^\gamma}{P^\gamma(x,y,z,T)}\right\}\frac{\partial C_1(x,y,z,\tau)}{\partial x}d\tau+$$
$$+\frac{\partial}{\partial y}\int_0^t D_L(x,y,z,T)\left\{1+\xi\frac{[\alpha_{2C}+C_1(x,y,z,\tau)]^\gamma}{P^\gamma(x,y,z,T)}\right\}\frac{\partial C_1(x,y,z,\tau)}{\partial y}d\tau+\frac{\partial}{\partial z}\int_0^t\frac{\partial C_1(x,y,z,\tau)}{\partial z}\times$$
$$\times D_L(x,y,z,T)\left\{1+\xi\frac{[\alpha_{2C}+C_1(x,y,z,\tau)]^\gamma}{P^\gamma(x,y,z,T)}\right\}d\tau+\Omega\frac{\partial}{\partial x}\int_0^t\nabla_S\mu\,(x,y,z,\tau)\int_0^{L_z}C_1(x,y,W,\tau)\,dW\times$$
$$\times\frac{D_S}{kT}d\tau+\Omega\frac{\partial}{\partial y}\int_0^t\frac{D_S}{kT}\nabla_S\mu\,(x,y,z,\tau)\int_0^{L_z}C_1(x,y,W,\tau)\,dW\,d\tau+f_C(x,y,z).\qquad(1d)$$

We determine average value of the second-order approximation of the considered concentration by using standard relation [12,13].

$$\alpha_{2C}=\frac{1}{\Theta L_x L_y L_z}\int_0^\Theta\int_0^{L_x}\int_0^{L_y}\int_0^{L_z}[C_2(x,y,z,t)-C_1(x,y,z,t)]\,dz\,dy\,dx\,dt.\qquad(6)$$

Substitution of the relation (1*e*) into the relation (6) gives us possibility to obtain zero value of the required average value α_{2C}.

Now we determine components of displacement vector by solution of the system of Eqs.(4). To determine components of displacement vector we used method of averaging of function corrections in standard form. Framework the approach we replace the above components in right sides of Eqs.(4) on their not yet known average values α_i. The substitution leads to the following results

$$\rho(z)\frac{\partial^2 u_{1x}(x,y,z,t)}{\partial t^2}=-K(z)\beta(z)\frac{\partial T(x,y,z,t)}{\partial x},\ \rho(z)\frac{\partial^2 u_{1y}(x,y,z,t)}{\partial t^2}=-K(z)\beta(z)\frac{\partial T(x,y,z,t)}{\partial y},$$
$$\rho(z)\frac{\partial^2 u_{1z}(x,y,z,t)}{\partial t^2}=-K(z)\beta(z)\frac{\partial T(x,y,z,t)}{\partial z}.$$

Integration of the left and right sides of the above equations leads to obtain relation for the second-order approximation of the first-order approximations of components of displacement vector. The first-order approximations could be written as

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

We obtain the second-order approximations of components of displacement vector could be calculated by replacement of the required components in the Eqs. (4) on the following sums α_i+ $u_i(x,y,z,t)$ [12-14]. This replacement leads to the following result

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

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

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

Integration of left and right sides of the above equations on time t leads to the following results

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

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

$$u_{2y}(x,y,z,t)=\frac{E(z)}{2\rho(z)[1+\sigma(z)]}\left[\frac{\partial^2}{\partial x^2}\int_0^t\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{\partial^2}{\partial x\partial y}\int_0^t\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta\right]+$$
$$+\frac{K(z)}{\rho(z)}\frac{\partial^2}{\partial x\partial y}\int_0^t\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{1}{\rho(z)}\frac{\partial^2}{\partial y^2}\int_0^t\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta\left\{\frac{5E(z)}{12[1+\sigma(z)]}+K(z)\right\}+$$
$$+\frac{1}{2\rho(z)}\frac{\partial}{\partial z}\left\{\frac{E(z)}{1+\sigma(z)}\left[\frac{\partial}{\partial z}\int_0^t\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{\partial}{\partial y}\int_0^t\int_0^\vartheta u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta\right]\right\}-K(z)\frac{\beta(z)}{\rho(z)}\times$$
$$\times\int_0^t\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{1}{\rho(z)}\left\{K(z)-\frac{E(z)}{6[1+\sigma(z)]}\right\}\frac{\partial^2}{\partial y\partial z}\int_0^t\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta-\frac{E(z)}{2\rho(z)}\times$$
$$\times\frac{1}{1+\sigma(z)}\left\{\frac{\partial^2}{\partial x^2}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{\partial^2}{\partial x\partial y}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta\right\}-\int_0^\infty\int_0^\vartheta T(x,y,z,\tau)\,d\tau\,d\vartheta\times$$
$$\times K(z)\frac{\beta(z)}{\rho(z)}-\frac{K(z)}{\rho(z)}\frac{\partial^2}{\partial x\partial y}\int_0^\infty\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta-\frac{1}{\rho(z)}\frac{\partial^2}{\partial y^2}\int_0^\infty\int_0^\vartheta u_{1x}(x,y,z,\tau)\,d\tau\,d\vartheta\{K(z)+$$
$$+\frac{5E(z)}{12[1+\sigma(z)]}\bigg\}-\frac{1}{\rho(z)}\left\{K(z)-\frac{E(z)}{6[1+\sigma(z)]}\right\}\frac{\partial^2}{\partial y\partial z}\int_0^\infty\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta+u_{0y}-\frac{1}{2\rho(z)}\times$$
$$\times\frac{\partial}{\partial z}\left\{\frac{E(z)}{1+\sigma(z)}\left[\frac{\partial}{\partial z}\int_0^\infty\int_0^\vartheta u_{1y}(x,y,z,\tau)\,d\tau\,d\vartheta+\frac{\partial}{\partial y}\int_0^\infty\int_0^\vartheta u_{1z}(x,y,z,\tau)\,d\tau\,d\vartheta\right]\right\}$$

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

In this paper we calculate the second-order approximations of concentration of material of epitaxial layer and components of displacement vector by using the method of averaging of function corrections. Recently we obtain, that the second-order approximation of a considered solution is usually enough good approximation to make qualitative analysis and to obtain some quantitative results. We compare all analytical results by numerical simulations.

3. DISCUSSION

In this section we used relations obtained in the previous section for analysis influence of diffusion of material of the epitaxial layer of heterostructure from Fig. 1 into the substrate on relaxation of mismatch-induced stress. Increasing of temperature of growth stimulates acceleration of the diffusion. The diffusion leads to spreading of interface between layers of heterostructure. At the same time presents of smooth interface gives us possibility to decrease value of mismatch-induced stress in neighborhood of the interface between layers of heterostructure. The qualitatively same results have been experimentally obtained in [14]. The decreasing one can obtain due to more gradual changing of properties of the heterostructure in direction, which is perpendicular to the interface of the heterostructure. The Fig. 2 shows dependences of components of displacement vector on coordinate deep into the heterostructure for sharp and smooth interfaces. Probably spreading of interface, which one can obtain during high-temperature growth, is a reason of decreasing of mismatch-induced stress. Decreasing of sharpness of the interface could be partially compensated by nonlinearity of diffusion of material of epitaxial layer in the substrate for the large quantity of diffusing material. Several spatial distributions of material of epitaxial layer in the substrate are presented in Fig. 3.

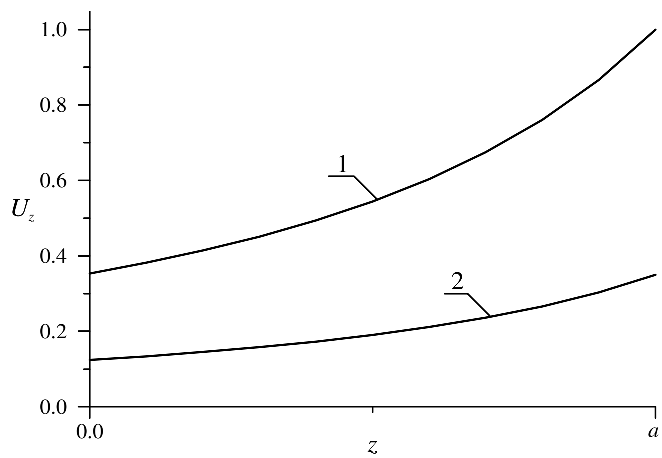

Fig.2. Normalized dependences of components of displacement vector u_z on coordinate z for sharp (curve 1) and smooth (curve 2) interfaces between layers of heterostructure

4. CONCLUSIONS

In this paper we discuss possibility to decrease value of mismatch-induced stress due to increasing of temperature of growth. At the same time one can find decreasing of sharpness of interface between layers of heterostructure. It has been discussed possibility at least partial compensation of decreasing of the sharpness.

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