Decreasing Value of Mechanical Stress in a Semiconductor Heterostructure by Using Modified Materials

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Abstract  In this paper we presented an approach to model and results of modeling of relaxation of mechanical stress in a heterostructure with porous epitaxial layer. We also presented an approach to model and result of modeling of modification of the porosity under influence of the mechanical stress. Due to the analysis of relaxation of mechanical stress and modification of porosity we obtain, that porosity of epitaxial layer leads to decreasing of value of mechanical stress in heterostructure. At the same time density of the epitaxial layer increases under influence of mechanical stress.

Keywords  Semiconductor Heterostructure, Porous Layer, Decreasing of Mechanical Stress, Increasing of Density of Porous Layer

PACS Numbers:  66.30.Lw, 62.20.Fe, 81.20.-n, 02.30.Jr, 02.30.Rz

1. Introduction

At the present time manufacturing of semiconductor devices usually based on using semiconductor heterostructures (SH) [1-4]. Lattice spacing assumes different values in different layers of SH. Due to the difference one can obtain mechanical stress in SH. To decrease the stress it could be used materials with as small as possible difference of lattice spacing. The second way to decrease the stress is using buffer layers for gradually decreasing of difference between lattice spacing in main layers of the SH. Framework the paper we consider alternative approach to decrease the mechanical stress in SH. The approach based on using porous layers in SH. At the same time we obtain decreasing of total volume of porous. We also introduce analytical approach to model relaxation of mechanical stress and modification of porosity at one time. We find in recently published literature modeling of this processes independently from each other and in more particular cases. For example, the authors of Ref. [5] have been considered only final stage of modification of porosity, when porous are almost spherical. On the other hand it has been experimentally shown in Ref. [6], that pores are not always spherical during their modification. In the Ref. [7] it has been considered only numerical simulation of mechanical stress without accounting relaxation of mechanical stress.

2. Statement of the Problem

We consider a SH, which consist of a substrate (S) with thickness $L$ and porous epitaxial layer (EL) with thickness $a$ (see Fig. 1). Let us determine displacement vector and distribution of vacancies in the SH. In this situation we assume, that pores consist of vacancies. The vacancies could migrate in the porous layer. In this situation with time (for example, during annealing [5,6]) small pores could decompose to vacancies and at the same time large pores could increases due to capturing of the free vacancies. We determine the characteristics with account temperature dependence, which gives appreciable contribution during doping of SH [8].
3. Method of Solution

We determine spatiotemporal distribution of concentrations of vacancies by solving the following equation \[7,9,10\]
\[
\frac{\partial V(x, y, z, t)}{\partial t} = \text{div} \left\{ D_v(z,T) \cdot \text{grad} \left[ V(x, y, z, t) \right] \right\} + \text{div} \left\{ \frac{D_{VS}(z,T)}{V T} \cdot \text{grad} \left[ \mu_1(x, y, z, t) \right] \right\} + \Omega \cdot \text{div} \left[ \frac{D_{VS}(z,T)}{k T} \cdot \text{grad} \mu_2(x, y, z, t) \right] V(x, y, W, t) dW
\]
(1)
with the initial and boundary conditions
\[
V(x, y, z, t) = \left\{ \begin{array}{ll}
V(x, y, z, 0) &= V_{\infty} \left( 1 + 2 \omega / k T \sqrt{x_1^2 + y_1^2 + z_1^2} \right) V(0, y, z, t) = 0; V(L_x, y, z, t) = 0; \\
V(x, y, 0, t) &= 0; V(x, y, L_z, t) = 0,
\end{array} \right.
\]
where \( S_1 \) is the surfaces of pores; \( S_2 \) is the surface of external boundary of porous region; \( \text{grad} \) and \( \text{div} \) are operators of surficial gradient and surficial divergence; \( V_0 \) is the modulus of normal velocity of movement of surface of growing or decreasing pore [10]; \( \omega = a^3 \), \( a \) is the atomic spacing; \( \Omega \) is the atomic volume; \( \Omega(x,y,z) \) is the temperature; \( k = 1.38 \times 10^{-23} \text{ J/K} \) is the Boltzmann constant; \( V \) is the molar volume; \( \mu_1(x,y,z,t) = R T \ln(V_2/V_1) \) [9], \( V_1 \) и \( V_2 \) is the initial and final volume of pores, \( R = 8.31 \text{ J/(mole·K)} \) is the molar gas constant; \( \mu_2(x,y,z,t) = \frac{E(z)}{\Omega} \cdot \frac{1}{2} \left[ \frac{\partial u_1(x,y,z,t)}{\partial x_j} + \frac{\partial u_1(x,y,z,t)}{\partial x_i} \right] \]
\[ - \epsilon_0 \delta_{ij} + \frac{\sigma(z)}{1 - 2 \sigma(z)} \left[ \frac{\partial u_k(x,y,z,t)}{\partial x_k} - 3 \epsilon_0 \right] - K(z) \chi(z) \left[ T(x,y,z,t) - T_0 \right] \delta_j E(z) \]
(2)
where \( \sigma \) is the Poisson coefficient; \( \epsilon_0 = (a_s - a_{EL})/a_{EL} \) is the mismatch strain, \( a_s, a_{EL} \) are lattice spacings for \( S \) and \( EL \), respectively; \( K \) is the modulus of uniform compression; \( \chi \) is the coefficient of thermal expansion; \( T_0 \) is the equilibrium temperature, which
coincide (for our case) with room temperature; \(E(z)\) is the Young modulus; \(\sigma_y\) 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 \[11\]; \(u_i\) are the components \(u_i(x,y,z,t)\), \(u_i(x,y,z,t)\) and \(u_i(x,y,z,t)\) of displacement vector \(\vec{u}(x, y, z, t)\); \(x_i\) are coordinates \(x, y, z\). Components of displacement vector could be obtained by solving of the following equations \[11\]

\[
\rho(z)\frac{\partial^2 u_i(x,y,z,t)}{\partial t^2} = \frac{\partial}{\partial x}\left[ \sigma_{xx}(x,y,z,t) + \frac{\partial \sigma_{xy}(x,y,z,t)}{\partial y} + \frac{\partial \sigma_{xz}(x,y,z,t)}{\partial z} \right]
\]

\[
\rho(z)\frac{\partial^2 u_y(x,y,z,t)}{\partial t^2} = \frac{\partial}{\partial x}\left[ \sigma_{yx}(x,y,z,t) + \frac{\partial \sigma_{yy}(x,y,z,t)}{\partial y} + \frac{\partial \sigma_{yz}(x,y,z,t)}{\partial z} \right],
\]

where \(\sigma_y = \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} - \delta_{ij} \frac{\partial u_k(x,y,z,t)}{\partial x_k} \right] \chi(z)K(z)\left[ T, -T(x,y,z,t) + K(z)\frac{\partial u_k(x,y,z,t)}{\partial x_k} \right];
\]

\(\rho(z)\) is the density of materials; \(\delta_{ij}\) is the Kronecker symbol. With account of the relation the last system of equation takes the form

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

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

\[
\frac{\partial^2 u_z(x,y,z,t)}{\partial x \partial z} - K(z)\chi(z)\frac{\partial T(x,y,z,t)}{\partial x},
\]

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

\[
K(z) + \frac{\partial}{\partial z} \left\{ \frac{E(z)}{2[1+\sigma(z)]} \left[ \frac{\partial u_i(x,y,z,t)}{\partial z} + \frac{\partial u_z(x,y,z,t)}{\partial y} \right] \right\} \right\} + \frac{\partial^2 u_y(x,y,z,t)}{\partial y^2} \left\{ \frac{5E(z)}{12[1+\sigma(z)]} + K(z) \frac{\partial^2 u_i(x,y,z,t)}{\partial x \partial y} \right. \]

\[
+ K(z) \right\} + \left\{ K(z) - \frac{E(z)}{6[1+\sigma(z)]} \right\} \frac{\partial^2 u_i(x,y,z,t)}{\partial y \partial z} + K(z) \frac{\partial^2 u_i(x,y,z,t)}{\partial x \partial y} (4)
\]
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Spatiotemporal distribution of temperature could be described by the second law of Fourier [12]

\[ c(T) \frac{\partial T(x, y, z, t)}{\partial t} = \text{div} \{ \lambda \cdot \text{grad} [T(x, y, z, t)] \} + p(x, y, z, t) \tag{5} \]

with the initial and boundary conditions

\[ \frac{\partial T(x, y, z, t)}{\partial x} \bigg|_{x=0} = \frac{\partial T(x, y, z, t)}{\partial x} \bigg|_{x=L_x} = 0; \quad \frac{\partial T(x, y, z, t)}{\partial y} \bigg|_{y=0} = \frac{\partial T(x, y, z, t)}{\partial y} \bigg|_{y=L_y} = 0; \]

\[ \frac{\partial T(x, y, z, t)}{\partial z} \bigg|_{z=0} = \frac{\partial T(x, y, z, t)}{\partial z} \bigg|_{z=L_z} = 0; \quad T(x, y, z, 0) = f_T(x, y, z) = \text{Tr}. \]

Here \( \lambda \) is the heat conduction coefficient. Value of the coefficient depends on materials of SH and temperature. Temperature dependence of heat conduction coefficient in most interest area could be approximated by the following function:

\[ \lambda(x, y, z, t) = \lambda_{ass}(x, y, z) [1 + \mu T^\sigma / T^0((x, y, z, t))] \]

where \( \lambda_{ass} \) is the heat capacitance; \( T^\sigma = c_{ass}[1 - \theta \exp(-r T(x, y, z, t) / T_d)] \) is the heat capacitance; \( T_d \) is the Debye temperature [12]. The temperature \( T(x, y, z, t) \) is approximately equal or larger, than Debye temperature \( T_d \) for most interesting for us temperature interval. In this situation one can approximately used:

\[ T(x, y, z, t) \approx c_{ass}. \]

First of all let us estimate spatiotemporal distribution of temperature. To make the estimations we transform the equation (5) with appropriate conditions to the following integral form

\[ T(x, y, z, t) = T(x, y, z, t) + \phi \left[ \int_0^t T(x, y, z, \tau) [T^\sigma(x, y, z, \tau) + \mu T^\sigma / T^0((x, y, z, t))] \frac{\partial T(x, y, z, \tau)}{\partial z} \, d\tau \right. \]

\[ \times \alpha_{ass}(z) - \int_0^z \alpha_{ass}(w) [T^\sigma(x, y, w, \tau) + \mu (\phi + 1) T^\sigma / T^0((x, y, z, t))] \left[ \frac{\partial T(x, y, w, \tau)}{\partial w} \right]^2 \, dw \, d\tau + A_s(x, y, z, t) \]

\[ + \frac{\partial}{\partial z} \left[ \int_0^t \frac{\partial \tilde{u}_s(x, y, z, \tau)}{\partial x} \, d\tau \right] \bigg|_{z=0} = \frac{\partial \tilde{u}_s(x, y, z, t)}{\partial z} \bigg|_{z=L_z} = 0; \quad \tilde{u}_s(x, y, z, 0) = \tilde{u}_0; \]

\[ \tilde{u}_s(x, y, z, \infty) = \tilde{u}_0. \]

Spatiotemporal distribution of temperature could be described by the second law of Fourier [12]

\[ c(T) \frac{\partial T(x, y, z, t)}{\partial t} = \text{div} \{ \lambda \cdot \text{grad} [T(x, y, z, t)] \} + p(x, y, z, t) \tag{5} \]

with the initial and boundary conditions

\[ \frac{\partial T(x, y, z, t)}{\partial x} \bigg|_{x=0} = \frac{\partial T(x, y, z, t)}{\partial x} \bigg|_{x=L_x} = 0; \quad \frac{\partial T(x, y, z, t)}{\partial y} \bigg|_{y=0} = \frac{\partial T(x, y, z, t)}{\partial y} \bigg|_{y=L_y} = 0; \]

\[ \frac{\partial T(x, y, z, t)}{\partial z} \bigg|_{z=0} = \frac{\partial T(x, y, z, t)}{\partial z} \bigg|_{z=L_z} = 0; \quad T(x, y, z, 0) = f_T(x, y, z) = \text{Tr}. \]
Here, \( A_s(x, y, z, t) = \int_0^\lambda \alpha_{ass}(w)T(x, y, w, \tau)\left[T^\phi(x, y, w, \tau) + \mu T_d^\phi\right]dwd\tau \)

\[-B_s(x, y, z, t) = \frac{1}{\varphi + 2} \int_0^\lambda T^{\phi+2}(x, y, w, \tau)dwd\tau + \tilde{P}(x, y, z, t) + F(x, y, z) \}

the replacement leads to the following result

\[ T_1(x, y, z, t) = \alpha_{T1} + \phi_1 \left[ \tilde{P}(x, y, z, t) - \frac{\alpha_{T1}^{\phi+2}}{\varphi + 2} + F(x, y, z) \right] \]

where \( \alpha_{T1}^{\phi+2} = 2\Theta L L_z (\Theta \bar{F} + \bar{P}) (\varphi + 2) \). Here \( F = \int_0^L \int_0^L (L_z - z) F^{\phi+2}(x, y, z) dzdxdy \), \( \bar{P} = \int_0^\Theta (\Theta - t) \int_0^L \int_0^L (L_z - z) \tilde{P}(x, y, z, t) dzdxdy \).

The second-order approximation of the temperature could be obtain by the following replacing \( T(x, y, z, t) -> \alpha_{T2} + T_1(x, y, z, t) \) in the right part of the Eq.(6). The relation is presented in the Appendix. Definition of the parameter \( \alpha_{T2} = (M_{T2} - M_{T1})/4L^2\Theta \) leads to obtaining equation to calculate the parameter. The equation is presented in the Appendix.

We used the second-order approximation for qualitative analysis and to obtain some quantitative estimation. In this situation we obtain main physical dependences and in some cases we also obtain enough good exactness of quantitative results [14,15]. Farther the distribution has been amended numerically.

Furthermore let us estimate components of displacement vector. In the common case exact solution of Eq. (4) is unknown. To obtain approximate solution we used method of averaging of functional corrections [13-15]. Let us previously transform the equations of the system (4) to the following integro-differential form.

Furthermore let us determine the first-order approximations of components of the displacement vector. To make the procedure we replace the components on their average values in the right sides of Eqs.(4), i.e. \( u_\beta(x, y, z, t) -> \alpha_{u\beta}, \beta = x, y, z \). The average values can be determine as

\[ \alpha_{u\beta 1} = M_{\beta 1} / 4L\Theta \]

where \( M_{\beta 1} = \int_0^\lambda \int_0^L \int_0^L u_\beta(x, y, z, t) dzdxdy \). The replacement gives us possibility to obtain

\[ u_{x1}(x, y, z, t) = \alpha_{x1} + \phi_1 \left[ G_{x0}(x, y, z, \infty) - G_{x1}(x, y, z, t) - \alpha_{x1} \Phi_{x0}(x, y, z, t) \right] \]
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Substitution of the obtained relations in Eqs. (7) gives us possibility to obtain the parameters $\alpha_{\beta i}$. The obtained results could be written as

\[
\alpha_{\beta i} = \Theta \frac{L_z [X_{\beta i 0} (\Theta) - X_{\beta i 2} (\Theta)]}{8 L^3 \int_0^L (L_z - z) \rho (z) d z},
\]

\[
\alpha_{\beta x 1} = \Theta \frac{L_z [X_{\beta x 1 0} (\Theta) - X_{\beta x 2} (\Theta)]}{8 L^3 \int_0^L (L_z - z) \rho (z) d z},
\]

\[
\alpha_{\beta z 1} = \Theta \frac{L_z [X_{\beta z 1 0} (\Theta) - X_{\beta z 2} (\Theta)]}{8 L^3 \int_0^L (L_z - z) \rho (z) d z},
\]

where

\[
X_{\beta i} (\Theta) = \int_0^\Theta \left( 1 + \frac{t}{\Theta} \right) \int_0^L \int_0^L (L_z - z) K (z) \chi (z) \frac{\partial T (x, y, z, t)}{\partial \beta} d z d y d x d t.
\]

The second-order approximations of the components of the displacement vector can be obtained by replacing of the functions $u_i (x, y, z, t)$ on the following sums: $u_i (x, y, z, t) = u_i (x, y, z, t) + \alpha_{\beta x i} (x, y, z, t)$, where $\alpha_{\beta x i} = (M_{x \beta i} - M_{x i}) / 4 L^3 \Theta$. Results of the replacement and calculations of parameters $\alpha_{\beta x i}$ are moved in the Appendix, because the results are bulky.

To determine the spatiotemporal distribution of vacancies let us transform the Eq. (1) to integral form. The integral form of the Eq.(1) is presented in the Appendix.

Furthermore we used method of averaging of functional corrections to solve the equations. The first- and the second-order approximation of vacancy concentration are also is presented in the Appendix.

In the following section we analyze relaxation of mechanical stress and spatiotemporal distribution of vacancies in the SH. The obtained relations give us possibility to analysed the relaxations demonstrably. Using numerical approaches gives us possibility to amend the obtained results.

4. Discussion

In this section we analyze relaxation of mechanical stress and spatiotemporal distribution of vacancies under the influence of the mechanical stress in SH. During the analysis we obtain, that for $\varepsilon_{0} > 0$ total volume of pores in EL decreases. At the same time volume of mechanical stress decreases. Probably, the decreasing of volume of pores is a consequence of compression of the EL under influence of the mechanical stress. At the same time with compression of the EL the mechanical stress also decreases. Probably, the decreasing is a consequence of increasing of density of atoms of the EL. The Fig. 2 shows dependences of component $u_i$ of displacement vector on coordinate $z$ for porous and nonporous epitaxial layers. The Fig. 3 shows dependences of vacancy concentrations on coordinate $z$ in stressed and unstressed epitaxial layers. The Fig. 2 shows, that mechanical stress in a SH with porous epitaxial layer decreases. Reason of the decreasing is increasing of density of porous epitaxial layer. In this situation it is possible decreasing of difference between lattice spacing in layers of the considered SH. The Fig. 3 shows increasing of density of porous epitaxial layer (i.e. decreasing of total volume of pores) under influence of relaxation of mechanical stress. Possible reason of the increasing of density of the epitaxial layer is migration of interstitials under influence of mechanical stress as under external force.
Figure 2. Normalized dependences of component $u_z$ of displacement vector on coordinate $z$ for nonporous (curve 1) and porous (curve 2) epitaxial layers. Here are $\varepsilon_0=0.02$, $E_1=0.1$, $E_2=0.12$, $K_1=0.5$, $K_2=0.6$, $\sigma_1=0.15$, $\sigma_2=0.17$. It should be noted, that we do not consider any concrete material. We consider some parameters to test our solution.

Figure 3. Normalized dependences of vacancy concentrations on coordinate $z$ in unstressed (curve 1) and stressed (curve 2) epitaxial layers. Here are $\varepsilon_0=0.02$, $E_1=0.1$, $E_2=0.12$, $K_1=0.5$, $K_2=0.6$, $\sigma_1=0.15$, $\sigma_2=0.17$. It should be noted, that we do not consider any concrete material. We consider some parameters to test our solution.

5. Conclusion

In this paper we analyzed relaxation of mechanical stress in a semiconductor heterostructure. It has been shown, that using of porous epitaxial layer gives us possibility to decrease value of mechanical stress in the structure. At the same time with decreasing of the value of the mechanical stress total volume of pores decreases under special condition. The condition has been determined in the paper.

Appendix

The second-order approximation of the temperature could be written as

$$T_2(x, y, z, t) = \alpha_{T2} + T_1(x, y, z, t) + \phi_1 \left( \int_0^t \left[ \alpha_{T2} + T_1(x, y, z, \tau) \right] \alpha_{T2} + T_1(x, y, z, \tau) \right) \mu \times$$

$$\frac{\partial T_1(x, y, z, \tau)}{\partial z} d \tau \alpha_{\text{ass}}(z) + A_{x21}(x, y, z, t) + A_{y21}(x, y, z, t) - B_{x1}(x, y, z, t) - B_{y1}(x, y, z, t) -$$
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Equation for calculation the parameter $\alpha_T$ could be written as

\[
-\int_0^t \int_0^w \alpha_{ass}(w) \left\{ [\alpha_{T2} + T_1(x, y, w, \tau)]^\phi + T_d^\phi \mu(\phi + 1) \right\} \left( \frac{\partial T_1(x, y, w, \tau)}{\partial w} \right)^2 dwd\tau + P(x, y, z, t) -
\]

\[
-\int_0^t \int_0^w \left[ [\alpha_{T2} + T_1(x, y, w, \tau)] \frac{\partial \left\{ [\alpha_{T2} + T_1(x, y, w, \tau)]^\phi + \mu T_d^\phi \right\}}{\partial w} \right] dwd\tau + F(x, y, z) -
\]

\[
-(\phi + 2)^{-1} \int_0^t [\alpha_{T2} + T_1(x, y, w, t)]^{\phi+2} d\tau.
\]

where $A_{g_{ij}}(x, y, z, t) = \int_0^t \int_0^w \alpha_{ass}(w) \left\{ [\alpha_{T1} + T_1(x, y, w, t)] \left\{ [\alpha_{T2} + T_1(x, y, z, t)]^\phi + \mu T_d^\phi \right\} \right\} \times \frac{\partial^2 T_j(x, y, w, t)}{\partial g^2} dwd\tau$, $B_{hi}(x, y, z, t) = \phi \mu T_d^\phi \int_0^t \int_0^w \alpha_{ass}(w) \left\{ \frac{\partial T_i(x, y, w, \tau)}{\partial h} \right\}^{2} dwd\tau$

Equation for calculation the parameter $\alpha_{T2}$ could be written as

\[
\int_0^t \int_0^w \int_0^L \alpha_{ass}(z) [\alpha_{T2} + T_1(x, y, z, t)] \left\{ [\alpha_{T2} + T_1(x, y, z, t)]^\phi + \mu T_d^\phi \right\} \frac{\partial T_1(x, y, z, t)}{\partial z} dwdzd\tau \times
\]

\[
(\Theta - t) d\tau - \int_0^t (\Theta - t) [\alpha_{ass}(z) [\alpha_{T2} + T_1(x, y, z, t)]^\phi + \mu (\phi + 1) T_d^\phi \right\} \frac{\partial T_1(x, y, z, t)}{\partial z} dwdzd\tau \times
\]

\[
\times \alpha_{ass}(z) [\alpha_{T2} + T_1(x, y, z, t)] \frac{\partial [\alpha_{T2} + T_1(x, y, z, t)]^\phi + \mu T_d^\phi \right\} \frac{\partial^2 T_j(x, y, z, t)}{\partial g^2} dwdzd\tau \times
\]

\[
\times \frac{\partial T_j(x, y, z, t)}{\partial z} (L_z - z) dwdzd\tau d\tau + \tilde{F} + \tilde{A}_{x+1} + \tilde{A}_{y+1} - \frac{1}{\phi + 2} \int_0^t \int_0^w [\alpha_{ass}(z) [\alpha_{T2} + T_1(x, y, z, t)]^\phi + \mu T_d^\phi \right\} \frac{\partial^2 T_j(x, y, z, t)}{\partial g^2} dwdzd\tau \times
\]

\[
\times (L_z - z) dwdzd\tau d\tau - B_{x+1} - B_{y+1} + \Theta F = 0,
\]

where $A_{g_{ij}} = \int_0^t (\Theta - t) [\alpha_{ass}(z) [\alpha_{T1} + T_1(x, y, z, t)]^\phi + \mu T_d^\phi \right\} \frac{\partial^2 T_j(x, y, z, t)}{\partial g^2} dwdzd\tau \times
\]

\[
\times \alpha_{ass}(z) (L_z - z) dwdzd\tau d\tau - B_{x+1} \times \Theta d\tau \mu T_d^\phi.
\]

The integro-differential equations for components of displacement vector

\[
u_t(x, y, z, t) = \nu_t(x, y, z, t) + \left\{ \frac{1}{6} C_{5-11}^{S-11} (x, y, z, t) + \frac{1}{2} C_{110}^{1101} (x, y, z, t) + \frac{1}{2} C_{110}^{1101} (x, y, z, t) \right\} -
\]

\[
- \frac{t}{6} C_{5-11}^{S-11} (x, y, z, \infty) - \frac{t}{2} C_{110}^{1100} (x, y, z, \infty) - \frac{t}{2} C_{110}^{1100} (x, y, z, \infty) - t D_0^{0 \infty} (x, y, z, t) +
\]
Here \( E_0 \) is the average value of the Young modulus. The integral form of the Eq. (1) could be written as

\[
\phi_2 = \frac{1}{2} C_{xyyzz}^{101} (x, y, z, t) - \frac{t}{2} C_{xyyzz}^{100} (x, y, z, \infty) + \frac{1}{6} C_{xyyzz}^{15-11} (x, y, z, t) - \\
- \frac{t}{6} C_{xyyzz}^{15-10} (x, y, z, \infty) - G_x (x, y, z, t) + t G_y (x, y, z, \infty) + D_{xyyzz}^{111} (x, y, z, t) - t D_{xyyzz}^{0} (x, y, z, \infty) + \\
+ \frac{1}{2} C_{xyyzz}^{0111} (x, y, z, t) - \frac{t}{2} C_{xyyzz}^{0111} (x, y, z, \infty) + H_x (x, y, z, \infty) - H_y (x, y, z, t) - \Phi_{y1} (x, y, z, t),
\]

\[
u_x (x, y, z, t) = \nu_x (x, y, z, t) + \phi_2 \left[ \frac{1}{2} C_{xyyzz}^{101} (x, y, z, t) - \frac{t}{2} C_{xyyzz}^{100} (x, y, z, \infty) + \frac{1}{6} C_{xyyzz}^{15-11} (x, y, z, t) - \\
- \frac{t}{6} C_{xyyzz}^{15-10} (x, y, z, \infty) - G_x (x, y, z, t) + t G_y (x, y, z, \infty) + D_{xyyzz}^{111} (x, y, z, t) - t D_{xyyzz}^{0} (x, y, z, \infty) + \\
+ \frac{1}{2} C_{xyyzz}^{0111} (x, y, z, t) - \frac{t}{2} C_{xyyzz}^{0111} (x, y, z, \infty) + H_x (x, y, z, \infty) - H_y (x, y, z, t) - \Phi_{y1} (x, y, z, t) \right],
\]

\[
u_z (x, y, z, t) = \nu_z (x, y, z, t) + \phi_2 \left[ \frac{1}{2} C_{xyyzz}^{101} (x, y, z, t) - \frac{t}{2} C_{xyyzz}^{100} (x, y, z, \infty) + \frac{1}{6} C_{xyyzz}^{15-11} (x, y, z, t) - \\
- \frac{t}{6} C_{xyyzz}^{15-10} (x, y, z, \infty) - G_x (x, y, z, t) + t G_y (x, y, z, \infty) + D_{xyyzz}^{111} (x, y, z, t) - t D_{xyyzz}^{0} (x, y, z, \infty) + \\
+ \frac{1}{2} C_{xyyzz}^{0111} (x, y, z, t) - \frac{t}{2} C_{xyyzz}^{0111} (x, y, z, \infty) + H_x (x, y, z, \infty) - H_y (x, y, z, t) - \Phi_{y1} (x, y, z, t) \right],
\]

Here \( C_{efghi}^{abcd} (x, y, z, t) = \left[ \int_{0}^{t} \int_{0}^{t} \int a \frac{\partial^2 u_x (x, y, w, \tau)}{\partial e \partial f} + b \frac{\partial^2 u_y (x, y, w, \tau)}{\partial g \partial h} + c \frac{\partial^2 u_z (x, y, w, \tau)}{\partial i \partial j} \right] \times \frac{E \left( \frac{d w}{1 + \sigma (w)} \right)}{(t - \tau) d \tau ,}
\]

\[
D_{abcdef} (x, y, z, t) = \left[ \int_{0}^{t} \int_{0}^{t} \int a \frac{\partial^2 u_x (x, y, w, \tau)}{\partial a \partial b} + b \frac{\partial^2 u_y (x, y, w, \tau)}{\partial c \partial d} + c \frac{\partial^2 u_z (x, y, w, \tau)}{\partial e \partial f} \right] \times \\
\times K \left( \frac{d w}{1 + \sigma (w)} \right) d \tau ,
\]

\[
H_{ai} (x, y, z, t) = \left[ \int_{0}^{t} \int_{0}^{t} \int a \frac{\partial^2 u_x (x, y, w, \tau)}{\partial \tau^2} \right] \rho \left( \frac{d w}{1 + \sigma (w)} \right) d \tau ,
\]

\[
\Phi_{\beta i} (x, y, z, t) = \left[ \int_{0}^{t} \int_{0}^{t} \int a \frac{\partial^2 u_x (x, y, w, \tau)}{\partial \tau^2} \right] \rho \left( \frac{d w}{1 + \sigma (w)} \right) d \tau ,
\]

\[
E_0 \text{ is the average value of the Young modulus. The integral form of the Eq. (1) could be written as}
\]

\[
V (x, y, z, t) = V (x, y, z, t) + \left\{ I_{x}^{011} (x, y, z, t) + I_{y}^{101} (x, y, z, t) + I_{z}^{110} (x, y, z, t) + J_{x}^{011} (x, y, z, t) +
\right.
\]

\[
+ D_{xyyzz}^{111} (x, y, z, t) + t G_x (x, y, z, t) + H_x (x, y, z, t) - t H_x (x, y, z, \infty) - \\
- \Phi_{x1} (x, y, z, t) \right\} \phi_2,
\]
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The first-order approximation of vacancy concentration could be written as

\[
V_1(x, y, z, t) = \alpha_{V_1} + \left\{ \begin{array}{l}
J_{10}^{111}(x, y, z, t) + J_{10}^{100}(x, y, z, t)
\end{array} \right\}
\]

\[
+ \frac{xyz(x + y + z + xz) L_x^{-1}}{L_y L_z (L_x L_y + L_y L_z + L_z L_x)} \left[ \begin{array}{l}
\alpha_{V_1} \left( \begin{array}{c}
\frac{1}{2}
\end{array} \right) L_x^2 L_y^2 L_z^2 - J_{10}^{011}(x, y, z, t) - J_{10}^{101}(x, y, z, t)
\end{array} \right]
\]

\[
- J_{00}^{011}(x, y, z, t) - F \left( L_x, L_y, L_z \right) - \alpha_{V_1} \tilde{K}_{011}(L_x, L_y, L_z, t) - \alpha_{V_1} \tilde{K}_{011}(L_x, L_y, L_z, t)
\]

\[
\cdot \frac{\alpha_{V_1}}{8} x^2 y^2 \times
\]

\[
x^2 + F(x, y, z),
\]

where \( \tilde{K}_{ijkl}(x, y, z, t) = \Omega L_z \int_{0}^{t} \int_{x}^{t} \int_{y}^{t} \int_{z}^{t} \frac{D_{yS}(w, T)}{k T} \nabla_{x} \mu_{y}(u, v, w, \tau) d W d w d(\tau - u) d t 关于}

\[
\alpha_{V_1} \text{ is the average value of vacancy concentration. The average value could be determined by the following relation}
\]

\[
\alpha_{V_1} = \frac{1}{\Theta L_x L_y L_z} \int_{0}^{t} \int_{x}^{t} \int_{y}^{t} \int_{z}^{t} V_1(x, y, z, t) d z d y d x d t
\]

Substitution of the first-order approximation of vacancies gives us possibility to obtain the average value in the final form.
The second-order approximation of vacancies concentration framework the method of averaging of functional correction takes the form

\[
\alpha_v = \left\lbrack \frac{L_x L_y L_z}{8} + \frac{L_x^2 L_y + L_y^2 L_z + L_z L_y^2}{8} \right\rbrack J_{21}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) + F \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \frac{L_y}{8} \left( \theta - x \right)^2 \times \\
\times \int_0^L \left( \frac{L_y - y}{L_y} \right)^2 \int_0^L \left( z - \omega \right)^2 f_r \left( x, y, z \right) d z d y d x - \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \\
- \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \\
- \Omega L_x \tilde{K}_{21}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \Omega L_x \tilde{K}_{21}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - L_x L_y L_z \Theta \times \\
\times \Theta / 72 \right\rbrack^{-1}.
\]

The parameter \( \alpha_v \) could be determined by using the following relation

\[
\alpha_v = \left\lbrack \frac{L_x L_y L_z}{8} + \frac{L_x^2 L_y + L_y^2 L_z + L_z L_y^2}{8} \right\rbrack J_{21}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) + F \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \frac{L_y}{8} \left( \theta - x \right)^2 \times \\
\times \int_0^L \left( \frac{L_y - y}{L_y} \right)^2 \int_0^L \left( z - \omega \right)^2 f_r \left( x, y, z \right) d z d y d x - \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \\
- \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \\
- \Omega L_x \tilde{K}_{21}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \Omega L_x \tilde{K}_{21}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - L_x L_y L_z \Theta \times \\
\times \Theta / 72 \right\rbrack^{-1}.
\]

The parameter \( \alpha_v \) could be determined by using the following relation

\[
\alpha_v = \left\lbrack \frac{L_x L_y L_z}{8} + \frac{L_x^2 L_y + L_y^2 L_z + L_z L_y^2}{8} \right\rbrack J_{21}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) + F \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \frac{L_y}{8} \left( \theta - x \right)^2 \times \\
\times \int_0^L \left( \frac{L_y - y}{L_y} \right)^2 \int_0^L \left( z - \omega \right)^2 f_r \left( x, y, z \right) d z d y d x - \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \\
- \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \\
- \Omega L_x \tilde{K}_{21}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \Omega L_x \tilde{K}_{21}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - L_x L_y L_z \Theta \times \\
\times \Theta / 72 \right\rbrack^{-1}.
\]

The parameter \( \alpha_v \) could be determined by using the following relation

\[
\alpha_v = \left\lbrack \frac{L_x L_y L_z}{8} + \frac{L_x^2 L_y + L_y^2 L_z + L_z L_y^2}{8} \right\rbrack J_{21}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) + F \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \\
- \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \frac{1}{4} J_{12}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \\
- \Omega L_x \tilde{K}_{21}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - \Omega L_x \tilde{K}_{21}^{10} \left( T_{x1}, T_{y1}, T_{z1}, \Theta \right) - L_x L_y L_z \Theta \times \\
\times \Theta / 72 \right\rbrack^{-1}.
\]
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The second-order approximations of components of displacement vector are

\[ u_{x2}(x, y, z, t) = \alpha_{x2} + u_{x1}(x, y, z, t) + \phi_1 \left[ \frac{1}{6} \cdot t \cdot C_{-1-11}^{1100}(x, y, z, 0) - \frac{t}{2} \cdot G_{x0}(x, y, z, 0) - G_{x1}(x, y, z, t) - \tilde{H}_{x11}(x, y, z, t) \right] + t \cdot \tilde{H}_{x11}(x, y, z, 0) - \Phi_{x1}(x, y, z, t) - \alpha_{x2} \cdot \Phi_{x0}(x, y, z, t) \]

\[ u_{y2}(x, y, z, t) = \alpha_{y2} + u_{y1}(x, y, z, t) + \phi_1 \left[ 0.5 \cdot C_{-15}^{1100}(x, y, z, 0) - t \cdot C_{150}(x, y, z, 0) \right] + 6^{-1} \left[ C_{-1-11}^{1100}(x, y, z, 0) - t \cdot C_{-15}^{1100}(x, y, z, 0) + C_{151}^{1101}(x, y, z, 0) - t \cdot C_{152}^{1101}(x, y, z, 0) \right] - G_{y1}(x, y, z, t) + t \cdot G_{y1}(x, y, z, 0) + D_{-y1}^{1100}(x, y, z, t) - t \cdot D_{y1}^{1100}(x, y, z, 0) - \tilde{H}_{y11}(x, y, z, t) + t \cdot \tilde{H}_{y01}(x, y, z, 0) - \alpha_{y2} \cdot \Phi_{y0}(x, y, z, t) - \Phi_{y1}(x, y, z, t) \right],

\[ u_{z2}(x, y, z, t) = \alpha_{z2} + \phi_1 \left[ 0.5 \cdot C_{-15}^{1100}(x, y, z, 0) - t \cdot C_{150}(x, y, z, 0) + C_{151}^{1101}(x, y, z, 0) - t \cdot C_{152}^{1101}(x, y, z, 0) \right] - 6^{-1} \left[ 3 \cdot C_{-1-11}^{1100}(x, y, z, 0) - C_{-1-15}^{1100}(x, y, z, 0) - C_{-1-150}(x, y, z, 0) - C_{-1-150}(x, y, z, 0) - t \cdot D_{y1}^{1100}(x, y, z, 0) - G_{y1}(x, y, z, t) + t \cdot G_{y1}(x, y, z, 0) + D_{-y1}^{1100}(x, y, z, t) - t \cdot D_{y1}^{1100}(x, y, z, 0) - \tilde{H}_{y11}(x, y, z, t) + t \cdot \tilde{H}_{y01}(x, y, z, 0) - \alpha_{y2} \cdot \Phi_{y0}(x, y, z, t) - \Phi_{y1}(x, y, z, t) \right],

\[ u_{z2}(x, y, z, t) = \alpha_{z2} + \phi_1 \left[ 0.5 \cdot C_{-15}^{1100}(x, y, z, 0) - t \cdot C_{150}(x, y, z, 0) + C_{151}^{1101}(x, y, z, 0) - t \cdot C_{152}^{1101}(x, y, z, 0) \right] - 6^{-1} \left[ 3 \cdot C_{-1-11}^{1100}(x, y, z, 0) - C_{-1-15}^{1100}(x, y, z, 0) - C_{-1-150}(x, y, z, 0) - C_{-1-150}(x, y, z, 0) - t \cdot D_{y1}^{1100}(x, y, z, 0) - G_{y1}(x, y, z, t) + t \cdot G_{y1}(x, y, z, 0) + D_{-y1}^{1100}(x, y, z, t) - t \cdot D_{y1}^{1100}(x, y, z, 0) - \tilde{H}_{y11}(x, y, z, t) + t \cdot \tilde{H}_{y01}(x, y, z, 0) - \alpha_{y2} \cdot \Phi_{y0}(x, y, z, t) - \Phi_{y1}(x, y, z, t) \right] \times \alpha_{z2} \right] + u_{z1}(x, y, z, t),\]
where 

\[ C_{e f g h i j k}^{a b c d}(x, y, z, t) = \int_0^z \int_0^z \left[ a \frac{\partial^2 u_{xk}(x, y, w, \tau)}{\partial e \partial f} + b \frac{\partial^2 u_{yk}(x, y, w, \tau)}{\partial g \partial h} + c \frac{\partial^2 u_{zk}(x, y, w, \tau)}{\partial i \partial j} \right] \times \]

\[ \times \frac{E(w)dw}{1 + \sigma(w)} (t - \tau)^d d \tau , \]

\[ \tilde{H}_{a j}(x, y, z, t) = \int_0^z (t - \tau)^{\frac{\partial^2 u_{aj}(x, y, w, \tau)}{\partial \tau^2}} \rho(w)dw d \tau . \]

Calculation of the parameters \( \alpha_{a u 2} \) leads to the following result

\[ \alpha_{a u 2} = L_z \left\{ \frac{1}{12} C_{x x y z 1}^{5-1-12}(L_x, L_y, L_z, \Theta) - \frac{\Theta^2}{12} C_{x x y z 1}^{5-1-10}(L_x, L_y, L_z, \infty) + \frac{1}{4} C_{x y y z z}^{11102}(L_x, L_y, L_z, \Theta) - \frac{\Theta^2}{4} C_{x y y z z}^{11100}(L_x, L_y, L_z, \infty) - \frac{1}{2} X_{y 2}(\Theta) + \frac{1}{2} \tilde{D}_{x y y z z}^{21}(L_x, L_y, L_z, \Theta) - \frac{\Theta^2}{2} \tilde{D}_{x y y z z}^{01}(L_x, L_y, L_z, \infty) + \frac{\Theta^2}{2} H_{x 01}(L_x, L_y, L_z, \infty) + \frac{\Theta^2}{2} X_{0 0}(\infty) - \frac{1}{2} H_{x 01}(L_x, L_y, L_z, \Theta) \right\} \right/ 4 \Theta L \tilde{H}_{y 01}(L_x, L_y, L_z, \Theta), \]

\[ \alpha_{u y 2} = L_z \left\{ \frac{1}{2} C_{x x y z z}^{11102}(L_x, L_y, L_z, \Theta) - \frac{\Theta^2}{2} C_{x y y z z}^{11100}(L_x, L_y, L_z, \infty) + \frac{1}{12} C_{x y y z z}^{1-15-12}(L_x, L_y, L_z, \Theta) + \frac{\Theta^2}{2} X_{y 0}(\infty) - \frac{\Theta^2}{12} C_{x y y z z}^{1-15-10}(L_x, L_y, L_z, \infty) + \frac{1}{2} C_{x y y z z}^{0110}(L_x, L_y, L_z, \Theta) - \tilde{D}_{x y y z z}^{0110}(L_x, L_y, L_z, \infty) \times \frac{\Theta^2}{2} \right\} \right/ 4 \Theta L \tilde{H}_{y 01}(L_x, L_y, L_z, \Theta), \]

\[ \alpha_{z 2} = \left\{ \frac{1}{2} C_{x y y z z}^{0112}(L_x, L_y, L_z, \Theta) - \frac{\Theta^2}{2} C_{x y y z z}^{01010}(L_x, L_y, L_z, \infty) + \frac{1}{2} C_{x y y z z}^{0112}(L_x, L_y, L_z, \Theta) - \frac{\Theta^2}{2} C_{x y y z z}^{10110}(L_x, L_y, L_z, \infty) + \frac{1}{2} \tilde{D}_{x y y z z}^{10112}(L_x, L_y, L_z, \Theta) + \frac{\Theta^2}{2} \tilde{D}_{x y y z z}^{10101}(L_x, L_y, L_z, \infty) \times \frac{\Theta^2}{2} \right\} \right/ 4 \Theta L \tilde{H}_{z 01}(L_x, L_y, L_z, \Theta), \]

where \( \Phi_{\beta j}(x, y, z, t) = \int_0^z \rho(w) \left[ u_{\beta j}(x, y, w, t) \right] dw \).
REFERENCES


