Coupled micro-macroscopic modeling of layered composites with finite deformations

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Abstract. A coupled micro- and macroscopic modeling of an incompressible layered composite material under finite deformations is performed based on the asymptotic homogenization method and universal semi-linear models. The deformation diagrams of the periodicity cell are calculated. A method for searching for effective transversally isotropic properties of LCM based on the obtained diagrams is considered. Cylindrical bending of an LCM plate is simulated using the model of a transversally isotropic medium. The microstresses in the periodicity cell are calculated based on the homogenized stresses. **Key words:** layered composite materials, macroscopic modeling, finite deformations.

1 Introduction

In various industries, composite materials are actively used, consisting of rubber-like or elastomeric matrices reinforced with fibers, dispersed particles, or fabric fillers. Such materials are of considerable interest, since they have successful combinations of properties, in particular, relatively high strength and a sufficiently large ultimate fracture strain due to the ability of rubbers to deform without fracture in the region of large deformations (up to 800–900%).

Due to the fact that the experimental determination of all the properties of composites with different reinforcement schemes requires rather complex experiments, along with experimental studies, it is important to build computational methods for finding the average (effective) nonlinear properties of composite materials, as well as models and methods that would allow one to determine not only general characteristics of such materials, but also locally describe the deformation processes occurring in them.

There are relatively simple algorithms and modeling methods that allow one to obtain simple analytical relationships for elastic effective characteristics. However, they do not allow them to be calculated most accurately in a mathematical sense.

Highly promising in this area is the method of asymptotic homogenization (AH) [1-6], which was proposed by N.S. Bakhvalov and G.P. Panasenko [1]. The asymptotic averaging method is a rigorous and widely used effective mathematical approach for describing the problems of deformation of structures made of composite materials, it gives an asymptotically correct representation of their solution. AH is also used to predict the effective

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properties of composites under finite strains [7–11]. Due to the nonlinearity of the problem of mechanics at finite deformations [12-15], the AH method encounters certain difficulties in implementation. The complexity of this method is justified by the possibility of obtaining a more accurate approximation of the desired solution compared to the theory using only effective properties.

However, the application of MAH to continuum media mechanics problems leads to the need to solve so-called local problems. Solving local problems is a complex and time-consuming process. If this method is used directly in solving macroscopic problems, for example, by the finite element method, then at each point (each node) it is necessary to solve a local problem on a periodicity cell, which leads to very large amounts of calculations. In other words, the problem of the connection between local problems in PC and a macroscopic problem is a serious problem that creates significant difficulties in numerical solution. In this regard, it is very important to develop an approximate method that would allow solving these problems separately.

2 Universal model of nonlinearly elastic isotropic composite components

Let us consider an inhomogeneous elastic solid medium (composite) V with finite deformations, which in the reference configuration $\overset{\circ}{K}$ has a periodic structure and it is possible to select a repeating element for it - a periodicity cell (PC) $\overset{\circ}{V}_{\xi}$, which consists of N components $\overset{\circ}{V}_{\alpha\xi}$, $\alpha = 1,...,N$. The Euler coordinates of each material point in the reference and actual configurations are denoted as x^k and $\overset{\circ}{x}^k$, they correspond to the Cartesian basis, and the Lagrangian coordinates are denoted as X^i. The latter are assumed to coincide with the Cartesian ones in the reference configuration, i.e. $X^i = \overset{\circ}{x}^i$. Each component of the composite will be assumed to be incompressible, obeying the universal class model B_n, according to the classification proposed in [16], the following constitutive relations hold for it

$$\overset{(n)}{\mathbf{T}} = -\frac{p}{n-III}\overset{(n)}{\mathbf{G}}^{-1} + \mu\left(n-III\right)^2\left(\left(\frac{1+\beta}{n-III} + \left(1-\beta\right)I_1\left(\overset{(n)}{\mathbf{G}}\right)\right)\mathbf{E} - \left(1-\beta\right)\overset{(n)}{\mathbf{G}}\right) \quad (1)$$

where $\overset{(n)}{\mathbf{T}}$ is the energy stress tensor [17], $\overset{(n)}{\mathbf{G}}$ is the energy measure of strain [17], which is expressed in terms of the strain gradient $\mathbf{F}$

$$\overset{(n)}{\mathbf{G}} = \frac{1}{n-III}(\mathbf{F}^T \cdot \mathbf{F})^{\frac{n-III}{2}}, \quad n = I, II, IV, V, \quad (2)$$

$\overset{(n)}{\mathbf{G}}^{-1}$ is inverse tensor, $I_1(\overset{(n)}{\mathbf{G}})$ is the first principal invariant (trace) of the tensor $\overset{(n)}{\mathbf{G}}$, $\mathbf{E}$ is metric tensor, p is hydrostatic pressure, μ и β are the elastic constants of the component, n is the number of the energy pair, which takes the following values: $n = I, II, IV, V$.

The Piola-Kirchhoff stress tensor $\mathbf{P}$ using relations (1) is calculated as follows

$$\mathbf{P} = {}^4\overset{(n)}{\mathbf{E}}{}^0 \cdot\cdot \overset{(n)}{\mathbf{T}} \tag{3}$$

where ${}^4\overset{(n)}{\mathbf{E}}{}^0$ is energy equivalence tensor [17], dependent only on the strain gradient $\mathbf{F}$.

3 Universal model of a nonlinearly elastic transversally isotropic composite

According to the AH method, for the composite as a whole, averaged constitutive relations are formulated that connect the averaged energy stress tensors $\overset{(n)}{\overline{\mathbf{T}}}$ and the averaged energy strain measures $\overset{(n)}{\overline{\mathbf{G}}}$.

Since the properties of a layered composite material do not change upon rotation in a plane parallel to the LCM layers, it can be considered a transversely isotropic medium. In addition, since, as has been proven, the LCM, which consists of incompressible phases, is itself an incompressible medium, the material under consideration can be described using universal models of incompressible transversely isotropic media.

The most general form of such models is the representation in tensor bases.

$$\overset{(\mathrm{n})}{\overline{\mathbf{T}}} = -\frac{\overline{p}}{n-III}\overset{(\mathrm{n})}{\overline{\mathbf{G}}}{}^{-1} + \sum_{\gamma=1}^{4}\varphi_\gamma \mathbf{I}_{\gamma\mathbf{G}} \tag{4}$$

We choose the representation of the Helmholtz free energy, which, in addition to the model number, depends on nine parameters, in the following form:

$$\overset{\circ}{\rho}\psi = \overset{\circ}{\rho}\psi_0 + \frac{1}{2}\Big(l_{11}\left(I_1-k_1\right)^{2n_1} + 2l_{12}\left(I_1-k_1\right)^{n_1}\left(I_2-k_2\right)^{n_2} + l_{22}\left(I_2-k_2\right)^{2n_2}\Big) + \\ + l_{33}\left(I_3-k_3\right)^{n_3} + l_{44}\left(I_4-k_4\right)^{2n_4} \tag{5}$$

Here we denote the invariants

$$I_1 = \left(\mathbf{E}-\mathbf{c}_3^2\right)\cdot\cdot\overset{(\mathrm{n})}{\mathbf{G}} \tag{6}$$

$$I_2 = \mathbf{c}_3^2\cdot\cdot\overset{(n)}{\mathbf{G}} \tag{7}$$

$$I_3 = \left(\left(\mathrm{E}-\mathbf{c}_3^2\right)\cdot\overset{(n)}{\mathbf{G}}\right)\cdot\cdot\left(\mathbf{c}_3^2\cdot\overset{(n)}{\mathbf{G}}\right) \tag{8}$$

$$I_4 = \overset{(n)}{\mathbf{G}}{}^2\cdot\cdot\mathbf{E} - I_2{}^2 + 2I_3 \tag{9}$$

$\overset{(n)}{\overline{\mathbf{G}}}$ is the averaged energy measure of deformation expressed in terms of the averaged strain gradient of the composite according to a formula similar to (2)

$$\overset{(n)}{\overline{\mathbf{G}}} = \frac{1}{n-III}(\overline{\mathbf{F}}^T \cdot \overline{\mathbf{F}})^{\frac{n-III}{2}}, n = I, II, IV, V. \tag{10}$$

The factors φ_γ in (7) are derivatives of the elastic potential $\varphi_\gamma = \rho\partial\psi / \partial I_\gamma$ and have a form

$$\begin{gathered} \varphi_1 = n_1 l_{11}\left(I_1 - k_1\right)^{2n_1-1} + n_1 l_{12}\left(I_1 - k_1\right)^{n_1-1}\left(I_2 - k_2\right)^{n_2}, \\ \varphi_2 = n_2 l_{22}\left(I_2 - k_2\right)^{2n_2-1} + n_2 l_{12}\left(I_1 - k_1\right)^{n_1}\left(I_2 - k_2\right)^{n_2-1}, \\ \varphi_3 = n_3 l_{33}\left(I_3 - k_3\right)^{n_3-1} \end{gathered} \tag{11}$$

$$k_1 = \frac{2}{n-III},\ k_2 = \frac{1}{n-III},\ k_3 = 0,\ k_4 = \frac{2}{\left(n-III\right)^2} \tag{12}$$

l_{11}, l_{12}, l_{22}, l_{44}, n_1, n_2, n_4 are the constants of the model of a transversally isotropic medium (composite).

For an inhomogeneous medium, we consider the problem of nonlinear elasticity theory in the Lagrangian description in the general formulation using universal models - models of the class B_n, proposed in [17] for compressible media with finite strains.

$$\overset{\circ}{\nabla}\cdot \mathbf{P} + \overset{\circ}{\rho}\mathbf{f} = \mathbf{0}, \quad X^i \in \overset{\circ}{V} \tag{13}$$

$$\mathbf{P} = \overset{(n)}{\mathrm{F}}{}^0(\mathbf{F}, X^i), \quad X^i \in \overset{\circ}{V} \cup \overset{\circ}{\Sigma} \tag{14}$$

$$\mathbf{F} = \mathbf{E} + \overset{\circ}{\nabla} \otimes \mathbf{u}, \quad X^i \in \overset{\circ}{V} \cup \overset{\circ}{\Sigma} \tag{15}$$

$$\overset{\circ}{\mathbf{n}}\cdot[\mathbf{P}] = \mathbf{0}, \quad [\mathbf{u}] = \mathbf{0}, \quad X^i \in \overset{\circ}{\Sigma}_{\alpha\beta} \tag{16}$$

$$\overset{\circ}{\mathbf{n}}\cdot \mathbf{P} = \mathbf{t}_e, \quad X^i \in \overset{\circ}{\Sigma}_1, \quad \mathbf{u} = \mathbf{u}_e, \quad X^i \in \overset{\circ}{\Sigma}_2 \tag{17}$$

Here (13) is the equilibrium equation, (14) are the constitutive relations of the nonlinear elastic medium, (15) is the kinematic relation, (16) are the conditions for ideal contact on the interfaces $\overset{\circ}{\Sigma}_{\alpha\beta}$ α^{th} and β^{th} composite components, (17) are the boundary conditions on parts $\overset{\circ}{\Sigma}_1$ and $\overset{\circ}{\Sigma}_2$ of the outer surface of the composite $\left(\overset{\circ}{\Sigma}_1 \cup \overset{\circ}{\Sigma}_2 = \partial\overset{\circ}{V}\right)$.

In expression (16) $[P^{ij}]$ is the function jump at the interface $\overset{\circ}{\Sigma}_{\alpha\beta}$ between the composite components.. All components of vectors and tensors are assigned to a fixed orthonormal basis $\mathbf{e}_k$ – - the reference configuration $\overset{\circ}{K}$.

Note that there is a connection between the Cauchy and Piola–Kirchhoff stress tensors

$$\mathbf{P} = \sqrt{\frac{g}{\overset{\circ}{g}}}\mathbf{F}^{-1} \cdot \mathbf{T}, \tag{18}$$

and therefore, having calculated one of them, we can consider the second one to be known, given the knowledge of the strain gradient.

4 Asymptotic solution of the problem of the nonlinear theory of elasticity

The idea of the asymptotic averaging method is based on combining the solution of local problems defined at the level of structural inhomogeneity of the material with the solution of a global problem (macro level) for an equivalent homogeneous medium.

Let us consider the case of a layered composite, which in the reference configuration is a system of parallel layers orthogonal to the direction OX^3, and periodically repeating in such a way that it is possible to introduce a periodicity cell (PC) - a set of a finite number of layers N with a total thickness ℓ.

The use of the asymptotic method involves the construction of asymptotic expansions of the functions included in the problem in terms of a small parameter equal to the ratio of the characteristic size of the periodicity cell to the characteristic size of the entire composite material.

We introduce a small parameter $\kappa = \ell/L << 1$, as a ratio of characteristic size ℓ of the PC to the characteristic size L of the whole composite (in reference configuration), and also introduce local Lagrangian coordinates ξ^i in $\overset{\circ}{K}$, which are related to the X^i as follows:

$$\xi^i = \frac{\bar{X}^i}{\kappa}, \quad \bar{X}^i = \frac{X^i}{L} \tag{19}$$

It is assumed that the local coordinates in the PC vary in the range $-1/2 \le \xi^i \le 1/2$. Due to the periodicity of the composite structure, all functions $\Omega(\xi^i, X^i)$, describing the motion of the composite components, including constituting relations (14), are periodic functions of ξ^i and are depending on the global Lagrangian coordinates X^i. Asymptotic expansions of the functions $\Omega(\xi^i, X^i)$ with respect to a small parameter are constructed

$$\Omega(\xi^i, X^i) = \Omega^{(0)}(X^i, \xi) + \kappa\Omega^{(1)}(X^i, \xi) + o(\kappa), \tag{20}$$

where $o(\kappa)$ are terms having a higher order of smallness compared to $\kappa\Omega^{(1)}(X^i, \xi)$.

In addition, the averaging of such functions over the PC is introduced:

$$\langle \Omega \rangle = \int_{\overset{o}{V}_\xi} \Omega d \overset{o}{V}_\xi \, . \tag{21}$$

The AH method also formulates a local problem of nonlinear elasticity in PC, as a result of solving which we find tensor relationships between the strain gradient in each component of the composite and the averaged strain gradient.

From the solution of local AH problems, we have four series of curves corresponding to uniaxial and biaxial tension

$$T_{11} = T^{(э)}{}_{11}\left(k_1\right) \tag{22}$$

$$T_{33} = T^{(э)}{}_{33}\left(k_3\right) \tag{23}$$

$$\begin{cases} T_{11} = T^{(э)}{}_{11}\left(k_1, k_2\right) \\ T_{22} = T^{(э)}{}_{22}\left(k_1, k_2\right) \end{cases} \tag{24}$$

$$\begin{cases} T_{11} = T^{(э)}{}_{11}\left(k_1, k_3\right) \\ T_{33} = T^{(э)}{}_{33}\left(k_1, k_3\right) \end{cases} \tag{25}$$

For an each specific set $\mathrm{C} = \{l_{11}, l_{12}, l_{22}, l_{44}, n_1, n_2, n_4\}$ the corresponding curves for a transversally isotropic material can be constructed, which we will call theoretical.

The problem of finding parameters $\mathrm{C} = \{l_{11}, l_{12}, l_{22}, l_{44}, n_1, n_2, n_4\}$ is formulated as a problem of minimizing some estimate of the deviation characterizing the discrepancy between the theoretical diagram for a specific set of parameters and the corresponding experimental one.

$$\min_{\mathrm{C}} R\left(T, T^{(э)}\right) \tag{26}$$

As an example of such an estimate, we present

$$R_2\left(T, T^{(э)}\right) = \sum_{\omega=1}^{N} \sum_{\alpha,\beta} \left(T_{\alpha\beta} - T^{(э)}_{\alpha\beta}\right)^2_{\omega} \tag{27}$$

Hera ω are numers of points at the points on the strain diagram.

5 Calculation of the parameters of the model of an effective layered composite material as a transversally isotropic medium

Calculations were carried out according to the developed method for a layered composite, the PC of which is consisted of two materials: rubber and polyurethane. The strain diagrams obtained using a numerical "experiment" (based on the direct solution of local problems in PC) for models and using approximation based on the effective transversal isotropic properies (ETIP) model are presented in Fig. 1a-1f

The approximation error of the considered "experimental" data was 10-12%.

Also, the effective elastic characteristics of the SCM from three layers were calculated (as a transversely isotropic medium).

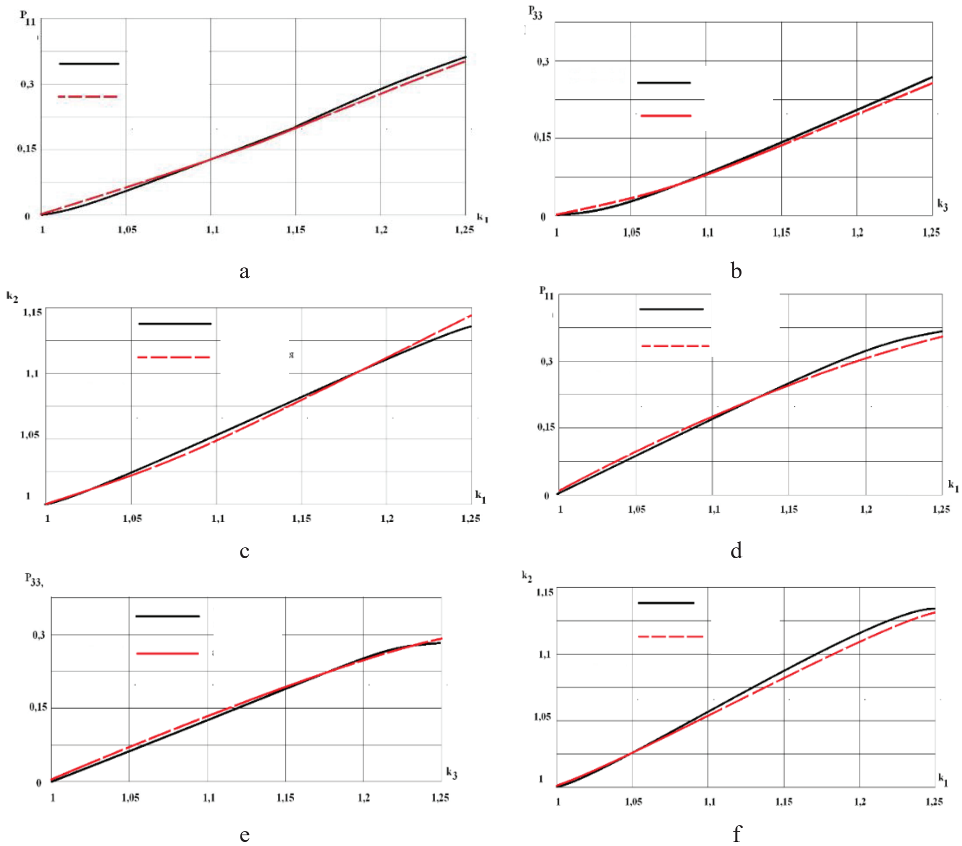

Fig. 1. Approximation of a numerical "experiment" - deformation diagrams for uniaxial deformation of a plate using the ETIP model for a two-layer rubber-polyurethane LCM.

According to the found parameters of the model, deformation diagrams were constructed. Comparative diagrams are shown in figures Fig. 2.

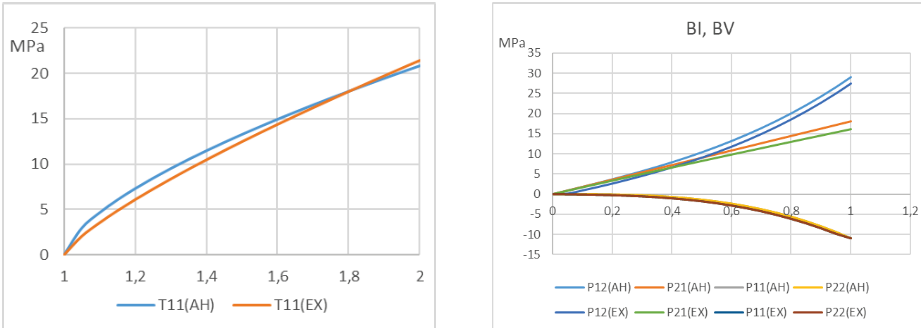

Fig. 2. Comparative diagram of shear deformation obtained by AH and from the model of a transversally isotropic medium.

The maximum relative errors in the resulting diagrams are 11% and 13%, respectively.

As a demonstration of the developed algorithm for solving problems of calculating stresses in layered composites at finite deformations, the problem of cylindrical bending of a layered composite plate is considered. A similar problem, but for homogeneous isotropic media with large deformations, was previously considered in the works of K.F. Chernykh [18].

Consider a laminated composite plate in the reference configuration $\mathring{K}$ (Fig 3). Volume $\mathring{V}$, corresponding to the plate in $\mathring{K}$ is described in in Cartesian coordinates $\mathring{x}^i$, $i=1,2,3$, as follows:

$$\mathring{K}:\mathring{V}=\left\{\mathring{x}^i \left| \mathring{x}_0^3-\frac{\mathring{h}_3}{2}<\mathring{x}_0^3<\mathring{x}_0^3+\frac{\mathring{h}_3}{2},\ -\frac{\mathring{h}_2}{2}<\mathring{x}_2<\frac{\mathring{h}_2}{2},\ -\frac{\mathring{h}_1}{2}<\mathring{x}_1<\frac{\mathring{h}_1}{2}\right.\right\} \tag{28}$$

where $\mathring{h}_i$ are the lengthes of the plate edges in $\mathring{K}$.

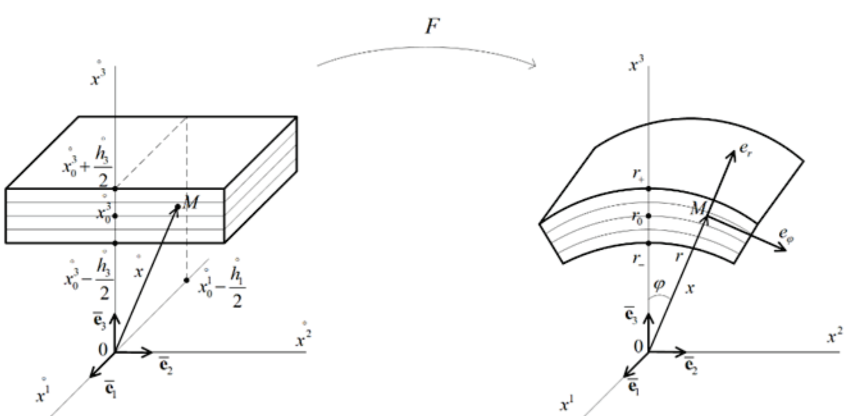

Fig. 3. Cylindrical bending of laminated plate.

Let us consider the law of motion (29) corresponding to the cylindrical bending of a plate into a cylindrical panel [19].

$$z=\mathring{x}^1,\quad \varphi=B\mathring{x}^2,\quad r=\sqrt{2A\mathring{x}^3} \tag{29}$$

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where A, B are constants.

The bending moment is defined as follows

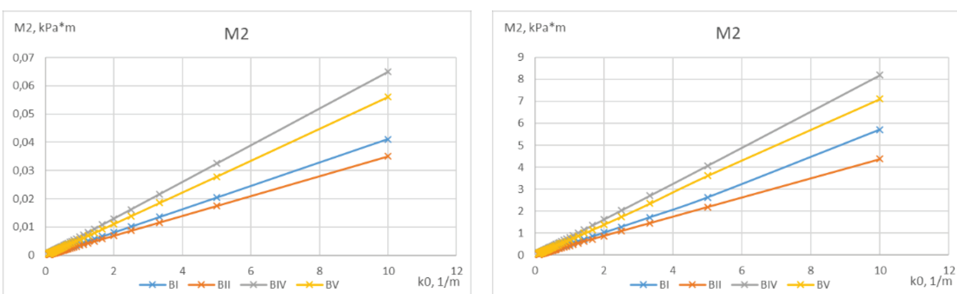
$$M_2 = \int_{r_-}^{r_+} r\overline{T}_{22} dr \tag{30}$$

Plate geometry: $L = 1м$, $\mathring{h}_3 = 0,01м$. When solving local problems by the AH method, the following elastic constants of the material were found

Table 1. Elastic constants of the material.

Model	l_{11}	l_{12}	l_{22}	l_{44}	n_1	n_2	n_4
B_I, B_V	22.0562	3.38152*10^{-13}	26.1652	4.73707	1	1	1
B_{II}, B_{IV}	13.8202	7.33581*10^{-14}	24.7085	4.97845	1	1	1

The dependences of the bending moment on the curvature calculated by formula (30) are shown in figures Fig. 4a and Fig 4b for two different panel thicknesses $\mathring{h}_3 = 0,01м$ and $\mathring{h}_3 = 0,05м$. With a 5 times increase in panel thickness, the torque value increases by 125 times for all models B_n. Thus, the dependence of the bending moment on the initial plate thickness is cubic, as for isotropic materials.



a b

Fig. 4. The dependence of the bending moment M2 from the bending curvature k_0, calculated by the formula (30), the panel thickness: a — $\mathring{h}_3 = 0,01m$, b — $\mathring{h}_3 = 0,05m$.

In figure Fig. 5 the averaged stresses in a transversally isotropic plate during bending. The distributions of the components of the Cauchy stress tensor $T_{22}(r)$ и $T_{33}(r)$ along the radial coordinate in are shown. Calculations were carried out for two plate thicknesses: $\mathring{h}_3 = 0,01m$ and $\mathring{h}_3 = 0,05m$. For a relatively thin plate, the distribution of the component $T_{22}(r)$ close to linear for all models B_n, which corresponds to the linear theory. For a thick plate, the distribution of the stress component $T_{22}(r)$ os nonlinear. For thick plates, the stress difference $T_{33}(r)$ for different models B_n is quite significant.

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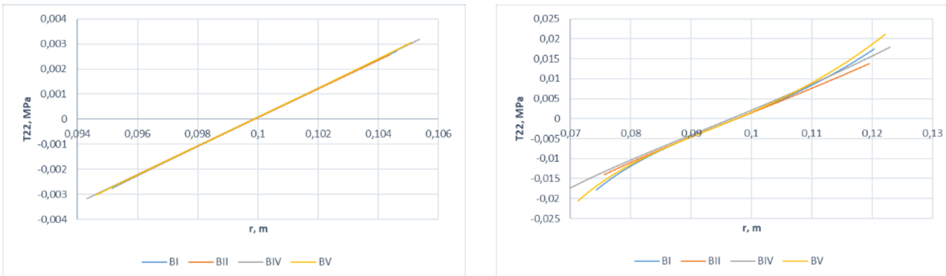

a b

Fig. 5 – Distribution of the component T_{22} of the Cauchy tensor along the radius r of the panel during the cylindrical bending $r_0 = 0{,}1m$ ($k_0 = 10m^{-1}$): a — $\mathring{h}_3 = 0{,}01m$, b — $\mathring{h}_3 = 0{,}05m$.

6 Conclusions

An algorithm for the numerical solution of problems on a periodicity cell for layered composite materials with finite deformations and using a complex of various universal models for compressible and incompressible media has been developed. A technique for constructing effective constitutive relations for transversally isotropic incompressible composites with finite strains is proposed based on the analytical approximation of series of numerical solution of local problems.

The problem of cylindrical bending of a layered composite plate is solved, which demonstrates the feasibility of the proposed method for calculating the stress-strain state of structures made of layered composite materials by separating the averaged problem of the nonlinear theory of elasticity of anisotropic media and local problems on a periodicity cell.

A variant of solving the problem of connectedness of micro- and macro-simulation problems by searching for ETIP constants that best approximate the behavior of the LCM obtained by preliminary micro-simulation based on AHM is demonstrated. The approach made it possible to solve the problem of macromodeling without resorting to the procedure for calculating local problems, while retaining the possibility of calculating microstresses.

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