FEATURES OF THE CONSTRUCTION OF THE STIFFNESS MATRIX OF THE SPATIAL HEXAGONAL FINITE ELEMENT FOR COMPOSITE MATERIAL WITH DISCRETE INCLUSIONS BASED ON THE MOMENT SCHEME

Shtanko H. I.

Postgraduate Student Zaporizhzhia National University Zhukovskoho str., 66, Zaporizhzhia, Ukraine orcid.org/0000-0002-8457-8269 sirouh177@gmail.com

Grebenyuk S. M.

Doctor of Technical Sciences, Professor, Head of the Department of Fundamental and Applied Mathematics Zaporizhzhia National University Zhukovskoho str., 66, Zaporizhzhia, Ukraine orcid.org/0000-0002-5247-9004 gsm1212@ukr.net

Key words: composite material, spherical and ellipsoidal inclusions, efficient elastic constants, finite element method, application package. An approach to numerical modeling of the stress-strain state of composite structures with discrete inclusions is presented in the paper. The finite element method is used as the main method, namely its modification – the moment finite-element scheme. The moment scheme, in contrast to the classic scheme of finite elements, allows to avoid such negative properties as not taking in consideration the rigid rotation of the finite element and "false" shear. If both the material of the matrix and the material of the reinforcing inclusions are weakly compressible, then problems arise due to the fact that some elastic constants approach very large values. The Taylor series expansion of the components of the displacement vector, the components of the strain tensor, and the volume change function is used in order to eliminate the mentioned shortcomings, after that, according to the moment scheme, certain sums are removed from these expansions.

Homogenization of the material with lamellar inclusions, a small proportion of spherical inclusions, and a large proportion of spherical inclusions is used for modeling the elastic properties of the composite. The chaotic nature of the location of inclusions after homogenization makes it possible to present a non-homogeneous composite material as a homogeneous quasi-isotropic one. The described approaches are used in the construction of the stiffness matrix of the spatial hexagonal finite element. The obtained expressions for the stiffness matrix are done in the software package for calculating structures from composite materials. The calculation of a thick-walled pipe under the action of internal pressure from a composite material with lamellar inclusions, a small proportion of spherical inclusions, and a large proportion of spherical inclusions was carried out using the software package. For different volume fractions of discrete inclusions, the numerical convergence of the results with different finite element meshes has been investigated, which shows great congruence with analytical solutions.

ОСОБЛИВОСТІ ПОБУДОВИ МАТРИЦІ ЖОРСТКОСТІ ПРОСТОРОВОГО ШЕСТИГРАННОГО СКІНЧЕННОГО ЕЛЕМЕНТА ДЛЯ КОМПОЗИЦІЙНОГО МАТЕРІАЛУ З ДИСКРЕТНИМИ ВКЛЮЧЕННЯМИ НА ОСНОВІ МОМЕНТНОЇ СХЕМИ

Штанько Г. І.

аспірант Запорізький національний університет вул. Жуковського, 66, Запоріжжя, Україна orcid.org/0000-0002-8457-8269 sirouh177@gmail.com

Гребенюк С. М.

доктор технічних наук, професор, завідувач кафедри фундаментальної та прикладної математики Запорізький національний університет вул. Жуковського, 66, Запоріжжя, Україна orcid.org/0000-0002-5247-9004 gsm1212@ukr.net

Ключові слова: композиційний матеріал, сферичні та еліпсоїдні включення, ефективні пружні сталі, метод скінченних елементів, пакет прикладних програм.

У роботі представлено підхід до чисельного моделювання напруженодеформованого стану конструкцій із композиційних матеріалів із дискретними включеннями. Як основний метод використано метод скінченних елементів, а саме його модифікацію – моментну схему скінченного елементу. Моментна схема, на відміну від класичної схеми скінченних елементів, дозволяє уникнути таких негативних властивостей, як неврахування жорсткого повороту скінченного елементу та «хибного» зсуву. У разі, якщо й матеріал матриці, й матеріал армуючих включень є слабкостисливими, то виникають проблеми, пов'язані з тим, що деякі пружні сталі прямують до дуже великих значень. Для усунення вказаних недоліків використовується розкладання в ряд Тейлора компонентів вектору переміщень, компонентів тензору деформацій та функції зміни об'єму після чого згідно моментній схемі певні доданки вилучаються з цих розкладань. Для моделювання пружних властивостей композиту використано гомогенізацію матеріалу із пластинчатими включеннями, малою часткою сферичних включень, великою часткою сферичних включень. Хаотичний характер розташування та орієнтації включень після гомогенізації дає можливість представити неоднорідний композиційний матеріал однорідним квазіізотропним. Описані підходи використано при побудові матриці жорсткості просторового шестигранного скінченного елементу. Отримані співвідношення для матриці жорсткості реалізовані у програмному пакеті для розрахунку конструкцій із композиційних матеріалів. За допомогою програмного пакету проведено розрахунок товстостінної труби під дією внутрішнього тиску з композиційного матеріалу з пластинчатими включеннями, малою часткою сферичних включень, великою часткою сферичних включень. Для різних об'ємних часток дискретних включень досліджено чисельну збіжність результатів при різних сітках розбиття на скінченні елементи, яка показує гарне співпадіння з аналітичними розв'язками.

Introduction. The progress of technologies for the production of structural materials leads to the appearance of new grades of materials, the mechanical properties of which are significantly different from the existing ones. The use of these materials in the manufacture of structures requires a description of their properties for design calculations. One of the common composite materials is a composite material reinforced with discrete inclusions of various shapes - spherical, ellipsoidal, needle-shaped, disk-shaped, and others. One of the calculations carried out is the strength calculation of the structure. Material heterogeneity due to the presence of discrete inclusions requires consideration of the geometry and properties of each discrete inclusion in the material when creating mathematical models. The creation of accurate mathematical models suitable for engineering calculations is possible only in the presence of a small number of inclusions, and for real materials, when the number of inclusions is significant, such models will be cumbersome and unsuitable for use. Another way of modeling is the homogenization of the material, and its representation as an imaginary homogeneous material with mechanical constants that are called effective. This approach allows avoiding the mathematical description of each inclusion in the material and making the mathematical model much simpler.

Both the complex geometry of the structure and the variety of processes occurring in the structure significantly limit the use of analytical methods when calculating the strength, hence numerical methods are used to solve the problem. The most common and universal method is the finite element method (FEM). But the traditional scheme of the finite element method has a number of negative properties that significantly slow down the convergence of solutions. Therefore, solving this problem leads to the emergence of various modifications of the method, which allow improving the accuracy of calculations. One of the effective modifications of the method is the moment finite-element scheme (MFES), developed for different groups of materials - isotropic, fibrous composites, weakly compressible, etc. This modification allows to avoid such imperfections of the traditional scheme as not taking into account the displacements of the finite element as a rigid whole and the "false" shear effect.

In the process of using the MFES, we will calculate the matrix of elastic constants using the effective elastic constants of the granular composite and will use an approach that takes into account the weak compressibility of the material, which will allow us to calculate both compressible and weakly compressible materials.

The application of the finite element method to the study of deformation processes of composites is given in a lot of studies. At the same time, such studies are carried out both at the micro and macro levels, as well as when modeling the interrelationship of the behavior of the composite material at the specified levels.

Literature review. In work [1], a computational procedure for modeling the microstructure of randomly reinforced composites with cylindrical or spherical-cylindrical inclusions is proposed. The proposed methodology combines the random sequential adsorption (RSA) algorithm for the preliminary modeling of the random location of inclusions with the subsequent application of the finite element method for the study of a representative volume of the composite material with inclusions, that have various characteristics of homogeneity and isotropy.

Modeling of the physical and mechanical properties of a polymer composite material using the spatial finite element method was carried out in [2]. ANSYS analysis software system was used to numerically determine the strength of materials randomly strengthened by spherical and cylindrical inclusions. A comparison was made with the results of full-scale tests.

Article [3] is devoted to the prediction of elastic and plastic constants composite material from polytetrafluoroethylene reinforced with aluminum. For this purpose, two types of 2D representative volumetric elements were developed and investigated based on the statistical analysis of microstructure images, taking into account the geometry and distribution of reinforcing particles and microvoids. The same microstructure is modeled and investigated in a three-dimensional setting using the finite element method. The obtained results indicate the effectiveness of the mentioned approaches.

The multilevel use of the finite element method at both the micro and macro levels is used in works [4; 5]. The accuracy and effectiveness of using FE² in models of the behavior of composite material under plastic deformation conditions based on the theory of small deformations were studied, and for the studied environment, decomposition by subdomains was used, each of which is related to the model of the composite material at the micro level [4]. The task of designing composite structures using the FE² finite element method based on two-level simultaneous optimization, which reduces the level of stress concentration and improves the stiffness properties of the composite with elliptical inclusions, was solved in [5].

The method of finite elements with its software implementations in CAD is also used directly for the calculation of structures from composite materials with mathematical models embedded in CAD. Thus, in work [6], ANSYS software based on the finite element method was used to estimate the deformations and stresses of a leaf spring made of composite material. Various combinations of composite materials, namely E-glass-epoxy, carbon-epoxy, boron-epoxy, and graphite-epoxy, were analyzed to select the optimal spring design.

In work [7], the finite element method was used to analyze composites in a wide variety of situations, namely, the behavior of materials was modeled depending on the theory, the type of material anisotropy, the law of failure criteria, etc. The finite element method was used for research at different levels of modeling – micro-, meso– and macro-levels. Different types of finite elements (plate, shell, and others) were used for modeling.

On the basis of the Abaqus software package and its extension using the Python programming code, examples of the calculation of composite materials for various problem statements are given, namely in the conditions of elasticity, viscoelasticity, the presence of damage, delamination, fatigue, strength studies, edge effects, etc. [8].

The moment finite-element scheme for the calculation of structures made of fibrous composite materials is presented in [9], where the spatial character of fiber reinforcement is taken into account.

Methods. In this work, we construct a stiffness matrix of a spatial finite element based on a moment scheme for calculating structures made of composite material reinforced with discrete inclusions. We also take into account the possibility of calculating composite materials with weakly compressible components.

Considering that the main goal is to study the spatial problems of the mechanics of composites, we build the stiffness matrix of the three-dimensional finite element. According to the geometric shape, spatial elements can be parallelepiped, triangular prisms and tetrahedrons, each of these elements has its own advantages and disadvantages. From the point of view of the symmetry of the approximating functions along the coordinate directions, among the proposed finite elements, the hexagonal element is generally more effective. Characteristic points are inherent in each element – the nodes of the finite element (as a rule, the corner points of the obtained model.

The stiffness matrix of the composite material with discrete inclusions using the MFES for the weakly compressible material is constructed. One of the most common geometric forms of a finite element is a parallelepiped, for which the same number of nodes along all coordinate directions is natural and, accordingly, there is symmetry in the approximating functions along the coordinates.

We get a discrete representation of the geometric area in the form of a collection of hexagonal finite elements, but their shape and size usually differ depending on one or another grid generator in case of applying the finite element method. It is unsuitable to perform mathematical operations and transformations for all types of forms when deriving the main ratios of the stiffness matrix. A more rational/ reasonable way is when a local coordinate system is introduced for each finite element, in which its shape and dimensions are displayed in a cube with a fixed side length (Fig. 1). Then, with the help of mathematical operators of transformation from one coordinate system to another, these relations are obtained in the global coordinate system, which describes the geometry of the structure and the boundary conditions. For the convenience of numerical integration according to Gauss quadrature formulas, let the length of the side of the cube be equal to 2. Let us number the eight nodes of the finite element as shown in fig. 1, we place the origin of the local coordinate system in the center of the cube.



Fig. 1. Mapping of a curvilinear parallelepiped finite element for a granular composite into a cubic one

Variational principles are one of the most wellfounded laws describing natural phenomena. To model the process of deformation of structures made of granular composites, we will use the variational principle of Lagrange. To do this, we need to determine the potential energy of the object under consideration. In the case of elastic deformation, this value can be written as follows:

$$\Pi^* = W^* - A^*, \tag{1}$$

where W^* - the energy of elastic deformation of the body, A^* - the work of external forces acting on the body.

According to Lagrange's variational principle, the potential energy Π^* variation is considered, which after discretization of the object is equal to the sum of the corresponding values for all finite elements:

$$\delta \Pi^* = \sum_{i=1}^n \delta W^{(i)} - \sum_{i=1}^n \delta A_i^{(i)},$$
(2)

here n – the number of finite elements.

This variational equation serves to form the system of solving equations of the finite element method. This procedure does not differ from the similar procedure in the traditional scheme of the finite element method, so let us focus on the obtaining of stiffness matrices of the finite element using the moment scheme. Let us write down the variation of the energy of elastic deformation $\delta W^{(i)}$ of an arbitrary *i*-th finite element by volume of *V* (redesignating $W^{(i)}$ for simplification by *W*):

$$\delta W = \iiint_{V} \sigma^{ij} \delta \varepsilon_{ij} dV,$$

and using the inverse form of generalized Hooke's law, we get

$$\delta W = \iiint_{\mathcal{V}} C^{ijkl} \varepsilon_{kl} \delta \varepsilon_{ij} dV,$$

in the matrix form, the last relation, taking into account the parity of the tangential stresses, will take the form

$$\delta W = \iiint_{v} \delta \left\{ \varepsilon_{ij} \right\}^{T} \left[C^{ijkl} \right] \left\{ \varepsilon_{kl} \right\} dV, \quad (3)$$

where $\{\varepsilon_{kl}\} = \{\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{33}, \varepsilon_{12}, \varepsilon_{13}, \varepsilon_{23}\}^T$ – vector of deformations, $[C^{ijkl}]$ – matrix of elastic constants of the material of the object.

As a result of homogenization of heterogeneous materials, we obtain a homogeneous material with effective mechanical characteristics. The material obtained after homogenization, depending on a number of initial parameters, such as the shape and location in space of reinforcing elements, properties of the matrix and fiber, can be classified as anisotropic (general case), orthotropic, transtropic materials, and, finally, as a quasi-isotropic material. The last case is characteristic of a granular composite material, that is, a quasi-isotropic material. A significant manifestation of anisotropic properties for such materials is not a frequent case – it is possible when, for example, reinforcing particles have a deterministically asymmetric shape and certain orientations when located in a composite.

Let us use the relation for the elastic constants of an isotropic (quasi-isotropic) material through the Lamé parameters λ , μ and the components of the metric tensor \hat{g} :

$$C^{ijkl} = \mu \left(g^{ik} g^{jl} + g^{il} g^{jk} \right) + \lambda g^{ij} g^{kl}$$

Considering that the effective elastic constants of a composite material are determined by the bulk modulus of elasticity *K* and the shear modulus *G*:

$$\mu = G, \lambda = K - \frac{2}{2}G$$

we will have

 $\delta W = \iiint_{v} \left(2Gg^{ik}g^{jl}\varepsilon_{kl} + \left(K - \frac{2}{3}G\right)\theta g^{ij} \right) \delta\varepsilon_{ij}dV,$ $\delta W = \iiint_{v} \left(2Gg^{ik}g^{jl}\varepsilon_{kl}\delta\varepsilon_{ij} + \left(K - \frac{2}{3}G\right)\theta\delta\theta \right) dV,$

or

where
$$\theta$$
 is the volume change function.

And expression (3) will take the form:

$$\delta W = \iiint_{\nu} \delta \left\{ \varepsilon_{ij} \right\}^{I} 2Gg^{ik}g^{jl} \left\{ \varepsilon_{kl} \right\} dV + \iiint_{\nu} \delta \left\{ \theta \right\}^{T} \left(K - \frac{2}{3}G \right) \left\{ \theta \right\} dV, \quad (4)$$

Thus, in fact, two independent elastic constants are needed to describe the elastic properties. Let us consider some approaches to their definition.

The following ratios can be used to determine effective elastic constant composite materials with discrete inclusions. For a composite material with a small volume fraction of spherical inclusions, we have the effective shear modulus [10]:

$$G = G^* \left(1 - \frac{15(1 - v^*)\left(1 - \frac{G^\circ}{G^*}\right)f}{7 - 5v^* + 2(4 - 5v^*)\frac{G^\circ}{G^*}} \right),$$
 (5)

effective bulk modulus

$$K = K^{*} + \frac{\left(K^{\circ} - K^{*}\right)f}{1 + \frac{\left(K^{\circ} - K^{*}\right)}{\left(K^{*} + \frac{4}{3}G^{*}\right)}},$$
(6)

here G^* , G° – are the shear modules of the material of the matrix and inclusion, respectively; K^* , K° – volume modules of matrix and inclusion material, respectively; v^* – Poisson's ratio of matrix material; f – the volume fraction of inclusions in the composite material.

For a composite material with a large volume fraction of spherical inclusions $(f \rightarrow 1)$ we have the effective shear modulus [10]:

$$G = G^{\circ} \left(1 - \frac{\left(1 - \frac{G^{*}}{G^{\circ}}\right) \left(7 - 5v^{*} + 2\left(4 - 5v^{*}\right)\frac{G^{\circ}}{G^{*}}\right) \left(1 - f\right)}{15\left(1 - v^{*}\right)} \right), \quad (7)$$

effective bulk modulus

$$K = K^{*} + \frac{\left(K^{\circ} - K^{*}\right)f}{1 + (1 - f)\frac{\left(K^{\circ} - K^{*}\right)}{\left(K^{*} + \frac{4}{3}G^{*}\right)}}.$$
(8)

For a composite material with a small volume fraction of lamellar inclusions, we have the effective shear modulus [10]:

$$G = G^{*} + \frac{\left(G^{\circ} - G^{*}\right)f}{1 + \frac{\left(G^{\circ} - G^{*}\right)}{\left(G^{*} + G^{*}\right)}}, \quad G' = \frac{G^{\circ}\left(9K^{\circ} + 8G^{\circ}\right)}{6\left(K^{\circ} + 2G^{\circ}\right)}, \tag{9}$$

effective bulk modulus

$$K = K^{*} + \frac{\left(K^{\circ} - K^{*}\right)f}{1 + \frac{\left(K^{\circ} - K^{*}\right)}{\left(K^{*} + \frac{4}{3}G^{\circ}\right)}}.$$
 (10)

An important procedure in the finite element method is the choice of the type of approximating functions, and how accurately the problem will be solved in the future depends on it. If the finite element is assumed to be isoparametric in the form of a parallelepiped with eight nodes (Fig. 1), then it is reasonable to choose a linear approximation in each of the three coordinate directions. In this case, according to the moment finite-element scheme for weakly compressible materials, three components characterizing the deformed state of the material are decomposed by local power functions of the form

$$\Psi^{(pqr)} = \frac{(x_1)^p (x_2)^q (x_3)^r}{p! q! r!},$$
(11)

here p = 0, ..., l; q = 0, ..., m; r = 0, ..., n – degrees of approximating functions in the corresponding coordinate directions; in the adopted law of approximation l = m = n = 1.

Then we will have for the components of the displacement vector:

$$u_{k'} = \sum_{p=0}^{l} \sum_{q=0}^{m} \sum_{r=0}^{n} \omega_{k'}^{(pqr)} \psi^{(pqr)}, \qquad (12)$$

for the components of the strain tensor

$$\varepsilon_{ij} = \sum_{p=0}^{L_{ij}} \sum_{q=0}^{M_{ij}} \sum_{r=0}^{M_{ij}} e_{ij}^{(pqr)} \psi^{(pqr)}, \qquad (13)$$

and volume change functions

$$\theta = \sum_{p=0}^{l-1} \sum_{q=0}^{m-1} \sum_{r=0}^{n-1} \xi^{(pqr)} \psi^{(pqr)}, \qquad (14)$$

where $\omega_{k'}^{(pqr)}$, $e_{ij}^{(pqr)}$, $\xi^{(pqr)}$ are the expansion coefficients of the components of the displacement vector, the deformation vector, and the volume change function, respectively.

In the vector-matrix form of the record, expressions (15) and (16) will take the form:

$$\boldsymbol{u}_{k'} = \left\{ \boldsymbol{\psi}_{ij} \right\} \left\{ \boldsymbol{\omega}_{k'} \right\}^T, \qquad (15)$$

$$\left\{\boldsymbol{\varepsilon}_{ij}\right\} = \left\{\boldsymbol{\psi}_{ij}\right\} \left\{\boldsymbol{e}_{ij}\right\}^{T}, \qquad (16)$$

$$\left\{\boldsymbol{\theta}\right\} = \left\{\boldsymbol{\Psi}_{\boldsymbol{\theta}}\right\} \left\{\boldsymbol{\xi}\right\}^{T}, \qquad (17)$$

where

$$\{\omega_{k'}\} = \left\{\omega_{k'}^{(000)}, \omega_{k'}^{(100)}, \omega_{k'}^{(010)}, \omega_{k'}^{(110)}, \omega_{k'}^{(001)}, \omega_{k'}^{(101)}, \omega_{k'}^{(011)}, \omega_{k'}^{(111)}\right\} - the vector of displacement expansion coefficients$$

the vector of displacement expansion coefficients,

$$\{\psi_{\theta}\} = \{\psi_{ij}\} = \{1, x_1, x_2, x_1, x_2, x_3, x_1, x_3, x_2, x_3, x_1, x_2, x_3\} -$$

the vector of power functions of the form (13),

$$\left\{\boldsymbol{e}_{ij}\right\} = \left\{\boldsymbol{e}_{ij}^{(000)}, \boldsymbol{e}_{ij}^{(100)}, \boldsymbol{e}_{ij}^{(010)}, \boldsymbol{e}_{ij}^{(110)}, \boldsymbol{e}_{ij}^{(001)}, \boldsymbol{e}_{ij}^{(101)}, \boldsymbol{e}_{ij}^{(011)}, \boldsymbol{e}_{ij}^{(111)}\right\} -$$

the vector of expansion coefficients of the volume change function,

$$\left\{\xi\right\} = \left\{\xi^{(000)},\xi^{(100)},\xi^{(010)},\xi^{(110)},\xi^{(001)},\xi^{(101)},\xi^{(011)},\xi^{(111)}\right\} \ -$$

the vector of expansion coefficients of the volume change function.

Substituting relations (18), (19) into (4), we obtain:

$$\delta W = \iiint_{v} \delta \left\{ e_{ij} \right\} \left\{ \psi_{ij} \right\}^{T} 2Gg^{ik}g^{jl} \left\{ \psi_{kl} \right\} \left\{ e_{kl} \right\}^{T} dV + \\ + \iiint_{v} \delta \left\{ \Theta \right\}^{T} \left(K - \frac{2}{3}G \right) \left\{ \Theta \right\} dV,$$
(18)

To determine the components $e_{ij}^{(pqr)}$, we will use the Cauchy relations that relate displacement to deformations:

$$\varepsilon_{ij} = \frac{1}{2} \left(\frac{\partial z_{m'}}{\partial x_j} u_{m',i} + \frac{\partial z_{m'}}{\partial x_i} u_{m',j} \right).$$
(19)

Differentiating (15), we have:

 u_k

$$\begin{aligned} u_{k',1} &= \omega_{k'}^{(100)} + \omega_{k'}^{(110)} \psi^{(010)} + \omega_{k'}^{(101)} \psi^{(001)} + \omega_{k'}^{(111)} \psi^{(011)} \\ u_{k',2} &= \omega_{k'}^{(010)} + \omega_{k'}^{(110)} \psi^{(100)} + \omega_{k'}^{(011)} \psi^{(001)} + \omega_{k'}^{(111)} \psi^{(101)} \\ \vdots &= \omega_{k'}^{(001)} + \omega_{k'}^{(101)} \psi^{(100)} + \omega_{k'}^{(011)} \psi^{(010)} + \omega_{k'}^{(111)} \psi^{(110)}. \end{aligned}$$
(20)

Then relations (19) will take the form:

$$\begin{split} & \varepsilon_{11} = \frac{\partial z_{k^{\cdot}}}{\partial x_{1}} \Big(\omega_{k^{\cdot}}^{(100)} + \omega_{k^{\cdot}}^{(110)} \psi^{(010)} + \omega_{k^{\cdot}}^{(101)} \psi^{(001)} + \omega_{k^{\cdot}}^{(111)} \psi^{(011)} \Big); \\ & \varepsilon_{22} = \frac{\partial z_{k^{\cdot}}}{\partial x_{2}} \Big(\omega_{k^{\cdot}}^{(010)} + \omega_{k^{\cdot}}^{(110)} \psi^{(100)} + \omega_{k^{\cdot}}^{(011)} \psi^{(001)} + \omega_{k^{\cdot}}^{(111)} \psi^{(101)} \Big); \\ & \varepsilon_{33} = \frac{\partial z_{k^{\cdot}}}{\partial x_{3}} \Big(\omega_{k^{\cdot}}^{(001)} + \omega_{k^{\cdot}}^{(101)} \psi^{(100)} + \omega_{k^{\cdot}}^{(011)} \psi^{(010)} + \omega_{k^{\cdot}}^{(111)} \psi^{(101)} \Big); \\ & \varepsilon_{12} = \frac{1}{2} \Big(\frac{\partial z_{k^{\cdot}}}{\partial x_{2}} \Big(\omega_{k^{\cdot}}^{(100)} + \omega_{k^{\cdot}}^{(110)} \psi^{(010)} + \omega_{k^{\cdot}}^{(101)} \psi^{(001)} + \omega_{k^{\cdot}}^{(111)} \psi^{(011)} \Big) + \\ & + \frac{\partial z_{k^{\cdot}}}{\partial x_{1}} \Big(\omega_{k^{\cdot}}^{(100)} + \omega_{k^{\cdot}}^{(110)} \psi^{(100)} + \omega_{k^{\cdot}}^{(101)} \psi^{(001)} + \omega_{k^{\cdot}}^{(111)} \psi^{(101)} \Big) \Big); \\ & \varepsilon_{13} = \frac{1}{2} \Big(\frac{\partial z_{k^{\cdot}}}{\partial x_{3}} \Big(\omega_{k^{\cdot}}^{(100)} + \omega_{k^{\cdot}}^{(110)} \psi^{(001)} + \omega_{k^{\cdot}}^{(101)} \psi^{(001)} + \omega_{k^{\cdot}}^{(111)} \psi^{(011)} \Big) \Big); \\ & \varepsilon_{23} = \frac{1}{2} \Big(\frac{\partial z_{k^{\cdot}}}{\partial x_{3}} \Big(\omega_{k^{\cdot}}^{(010)} + \omega_{k^{\cdot}}^{(110)} \psi^{(100)} + \omega_{k^{\cdot}}^{(011)} \psi^{(001)} + \omega_{k^{\cdot}}^{(111)} \psi^{(101)} \Big) \Big); \\ & \varepsilon_{24} = \frac{1}{2} \Big(\frac{\partial z_{k^{\cdot}}}{\partial x_{3}} \Big(\omega_{k^{\cdot}}^{(010)} + \omega_{k^{\cdot}}^{(110)} \psi^{(100)} + \omega_{k^{\cdot}}^{(011)} \psi^{(101)} + \omega_{k^{\cdot}}^{(111)} \psi^{(101)} \Big) \Big). \quad (21) \end{split}$$

Then the coefficients of the deformation vector $e_{ij}^{(pqr)}$ in expression (16) can be determined by the formula:

$$e_{ij}^{(pqr)} = \frac{\partial^{p+q+r}\varepsilon_{ij}}{\left(\partial x_1\right)^p \left(\partial x_2\right)^q \left(\partial x_3\right)^r} \bigg|_{x_1 = x_2 = x_3 = 0}.$$
 (22)

As a result, we will have the following ratios for the expansion coefficients $e_{ij}^{(pqr)}$:

$$e_{11}^{(pqr)} = \sum_{\mu\nu\eta}^{pqr} \omega_{k'}^{(\mu+1\nu\eta)} f_{(p+1-\mu q-\nu r-\eta)}^{k'};$$

$$e_{22}^{(pqr)} = \sum_{\mu\nu\eta}^{pqr} \omega_{k'}^{(\mu\nu+1\eta)} f_{(p-\mu q+1-\nu r-\eta)}^{k'};$$

$$e_{33}^{(pqr)} = \sum_{\mu\nu\eta}^{pqr} \omega_{k'}^{(\mu\nu\eta+1)} f_{(p-\mu q-\nu r+1-\eta)}^{k'};$$

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$$e_{12}^{(pqr)} = \frac{1}{2} \sum_{\mu\nu\eta}^{pqr} \left(\omega_{k'}^{(\mu\nu+1\eta)} f_{(p-\mu+1q-\nu r-\eta)}^{k'} + \omega_{k'}^{(\mu+1\nu\eta)} f_{(p-\muq-\nu+1r-\eta)}^{k'} \right);$$

$$e_{13}^{(pqr)} = \frac{1}{2} \sum_{\mu\nu\eta}^{pqr} \left(\omega_{k'}^{(\mu\nu\eta+1)} f_{(p-\mu+1q-\nu r-\eta)}^{k'} + \omega_{k'}^{(\mu+1\nu\eta)} f_{(p-\muq-\nu r-\eta+1)}^{k'} \right);$$

$$e_{23}^{(pqr)} = \frac{1}{2} \sum_{\mu\nu\eta}^{pqr} \left(\omega_{k'}^{(\mu\nu\eta+1)} f_{(p-\muq-\nu+1r-\eta)}^{k'} + \omega_{k'}^{(\mu\nu+1\eta)} f_{(p-\muq-\nu r-\eta+1)}^{k'} \right), \quad (23)$$

where the notation is entered

$$f_{(\mu\nu\eta)}^{k'} = \frac{\partial^{\mu+\nu+\eta} z_{k'}}{(\partial x_1)^{\mu} (\partial x_2)^{\nu} (\partial x_3)^{\eta}} \bigg|_{x_1 = x_2 = x_3 = 0}.$$
 (24)

To determine the coefficients (24), it is necessary to establish a connection between the global coordinate system z_k , and the local one associated with the finite element x_i . For an isoparametric finite element, this relationship will also be linear:

$$z_{k'} = \sum_{L=0}^{8} N_L(x_1, x_2, x_3) z_{k'}^L, \qquad (25)$$

where is the $z_{k'}^{L} - k'$ -th (k' = 1, 2, 3) coordinate of the L-node in the global coordinate system (L = 1, ..., 8), $N_L(x_1, x_2, x_3)$ - the approximating functions (shape functions) of the L node, which for a finite element with a linear law of approximation in all three directions are determined by the formula [10]:

$$N_{L} = \frac{1}{8} \left(1 + x_{1} x_{1}^{L} \right) \left(1 + x_{2} x_{2}^{L} \right) \left(1 + x_{3} x_{3}^{L} \right), \quad (26)$$

where x_i^L is the *i*-th coordinate (*i* = 1,2,3) of the *L*-th (*L* = 1,...,8) node in the local coordinate system associated with the finite element.

In more detail, the shape functions N_L for the nodes of the finite element can be written as follows:

$$N_{1} = \frac{1}{8} (1 - x_{1})(1 - x_{2})(1 - x_{3}), N_{2} = \frac{1}{8} (1 + x_{1})(1 - x_{2})(1 - x_{3}),$$
$$N_{3} = \frac{1}{8} (1 - x_{1})(1 + x_{2})(1 - x_{3}), N_{4} = \frac{1}{8} (1 + x_{1})(1 + x_{2})(1 - x_{3}),$$

$$N_5 = \frac{1}{8} (1 - x_1) (1 - x_2) (1 + x_3), N_6 = \frac{1}{8} (1 + x_1) (1 - x_2) (1 + x_3),$$

$$N_7 = \frac{1}{8} (1 - x_1) (1 + x_2) (1 + x_3), N_8 = \frac{1}{8} (1 + x_1) (1 + x_2) (1 + x_3). \quad (27)$$

Now let's return to relationship (24) for the coefficients of expansion of deformations $e_{ij}^{(pqr)}$, analyzing them, we can see that some of them contain coefficients $\omega_{k'}^{(pqr)}$ that are not included in the expansion of displacements (15). Therefore, the deformation expansion coefficients (24) containing at least one of the terms that are not included in the displacement expansion (15) should be removed from the expansion (24). Taking into account the mentioned rules of the moment finite-element scheme, the components of the vector of deformations will take the form:

$$\begin{split} \varepsilon_{11} &= e_{11}^{(000)} + e_{11}^{(010)} \psi^{(010)} + e_{11}^{(001)} \psi^{(001)} + e_{11}^{(011)} \psi^{(011)} ,\\ \varepsilon_{22} &= e_{22}^{(000)} + e_{22}^{(100)} \psi^{(100)} + e_{22}^{(001)} \psi^{(001)} + e_{22}^{(101)} \psi^{(101)} ,\\ \varepsilon_{33} &= e_{33}^{(000)} + e_{33}^{(100)} \psi^{(100)} + e_{33}^{(010)} \psi^{(100)} + e_{33}^{(110)} \psi^{(110)} ,\\ \varepsilon_{12} &= e_{12}^{(000)} + e_{12}^{(001)} \psi^{(001)} ,\\ \varepsilon_{13} &= e_{13}^{(000)} + e_{13}^{(010)} \psi^{(100)} ,\\ \varepsilon_{23} &= e_{23}^{(000)} + e_{23}^{(100)} \psi^{(100)} . \end{split}$$

The deformation expansion coefficients in (29) in vector-matrix form will take the form:

$$\left\{\boldsymbol{e}_{ij}\right\} = \left\{\boldsymbol{\omega}_{k'}\right\} \begin{bmatrix} F_{ij}^{k'} \end{bmatrix}.$$
(29)

In this expansion, the matrix $\begin{bmatrix} F_{ij}^{k^*} \end{bmatrix}$ is formed on the basis of (24) taking into account the removal of some coefficients according to the moment finite-element scheme.

The expansion coefficients of the volume change function are determined by the ratio:

$$\xi^{(\alpha\beta\gamma)} = \frac{\partial^{(\alpha+\beta+\gamma)} \varepsilon_{ij} g^{ij}}{\left(\partial x^{1}\right)^{\alpha} \left(\partial x^{2}\right)^{\beta} \left(\partial x^{3}\right)^{\gamma}} \bigg|_{x^{1} = x^{2} = x^{3} = 0} .$$
(30)

With the linear approximation of movements according to the moment finite-element scheme, the volume change function will take the form:

$$\theta = \xi^{(000)}.$$

In matrix form, expression (30) will be written as follows:

$$\{\xi\} = \{\omega_{k'}\} \Big[F_{\theta}^{k'} \Big]. \tag{31}$$

The matrix form of recording the variation of elastic deformation energy (19), taking into account (29), will take the form:

$$\delta W = \iiint_{v} \delta \{\omega_{k'}\} \Big[F_{ij}^{k'} \Big] \{\psi_{ij} \}^{T} 2Gg^{ik}g^{jl} \{\psi_{kl}\} \Big[F_{ij}^{m'} \Big]^{T} \{\omega_{m'}\}^{T} dV + \\ + \iiint_{v} \delta \{\omega_{k'}\} \Big[F_{\theta}^{k'} \Big] \{\psi_{\theta}\}^{T} \Big(K - \frac{2}{3} G \Big) \{\psi_{\theta}\} \Big[F_{ij}^{m'} \Big]^{T} \{\omega_{m'}\}^{T} dV, \quad (32)$$

And taking into account that some components of this sum can be taken beyond the sign of the triple integral, we will have:

$$\delta W = \delta \left\{ \omega_{k'} \right\} \left[F_{ij}^{k'} \right] \iiint_{v} \left\{ \psi_{ij} \right\}^{T} 2Gg^{ik}g^{jl} \left\{ \psi_{kl} \right\} dV \left[F_{ij}^{m'} \right]^{T} \left\{ \omega_{m'} \right\}^{T} + \delta \left\{ \omega_{k'} \right\} \left[F_{\theta}^{k'} \right] \iiint_{v} \left\{ \psi_{\theta} \right\}^{T} \left(K - \frac{2}{3}G \right) \left\{ \psi_{\theta} \right\} dV \left[F_{\theta}^{m'} \right]^{T} \left\{ \omega_{m'} \right\}^{T}, \quad (33)$$

or

$$\begin{split} \delta W &= \delta \left\{ \omega_{k'} \right\} \left[F_{ij}^{k'} \right] \left[H^{ijkl} \right] \left[F_{kl}^{m'} \right]^{T} \left\{ \omega_{m'} \right\}^{T} + \\ &+ \delta \left\{ \omega_{k'} \right\} \left[F_{\theta}^{k'} \right] \left[H^{\theta} \right] \left[F_{\theta}^{m'} \right]^{T} \left\{ \omega_{m'} \right\}^{T} , \end{split} \tag{34}$$

here

$$\left[H^{ijkl}\right] = \int_{-1-1-1}^{1} \int_{-1}^{1} 2Gg^{ik}g^{jl} \left\{\psi_{ij}\right\}^{T} \left\{\psi_{kl}\right\} \sqrt{g} dx_{1} dx_{2} dx_{3}, \quad (35)$$

$$\left[H^{\theta}\right] = \int_{-1-1-1}^{1} \int_{-1}^{1} \left(K - \frac{2}{3}G\right) \left\{\psi_{\theta}\right\}^{T} \left\{\psi_{\theta}\right\} \sqrt{g} dx_{1} dx_{2} dx_{3} \quad (36)$$

are the components of the matrix of elastic constants of an isotropic (quasi-isotropic) material, taking into account the metric of space.

In expansion (32), all components are defined, except for the displacement expansion coefficients, their determination makes it possible to write down the desired displacement function (15) and, therefore, to solve the problem. But these coefficients do not have visible mechanical meaning, so it is reasonable, as in the classic version of the finite element method, to move from them to the nodal values of displacements, which have a clear mechanical meaning.

Let us write the linear approximation of the components of the displacement vector u_k in the global coordinate system Oz1'z2'z3' for the hexagonal finite element through the nodal values of the displacements u_k^L and the shape functions $N_L(x_1, x_2, x_3)$:

$$u_{k'} = \sum_{L=0}^{8} N_L(x_1, x_2, x_3) u_{k'}^L,$$

here u_{k}^{L} – is the movement of the *L*-th node in the *k*-th direction in the global coordinate system, $N_{L}(x_{1}, x_{2}, x_{3})$ – is the shape function of the *L*-th node of the form (27).

Let us find the connection between the coefficients of displacements $\omega_k^{(pqr)}$ and the nodal values of displacements u_k^L by defining the matrix of transformations [A]. The matrix [A] describes the relationship between shape functions N_L and power functions $\psi^{(pqr)}$. Both of them are inherently a set of power functions, but when describing movements they are grouped in a combination in different ways, therefore, to find the matrix [A] that reflects this relationship, we use relation (15), on the other hand, (33) can be written as:

$$u_{k'} = \{N_L\} \{u_{k'}^L\}^T, \qquad (37)$$

where $\{u_{k}^{L}\} = \{u_{k}^{(1)}, u_{k}^{(2)}, u_{k}^{(3)}, u_{k}^{(4)}, u_{k}^{(5)}, u_{k}^{(6)}, u_{k}^{(7)}, u_{k}^{(8)}\}$ – is the vector of nodal displacements,

 $\{N_L\} = \{N_1, N_2, N_3, N_4, N_5, N_6, N_7, N_8\}$ – the vector of shape functions determined by formulas (27).

Comparing (11) and (27), we have the relation:

$$\{N_L\} = \{\Psi_{ij}\} [A]^T . \tag{38}$$

Considering the equality of the right-hand sides of relations (15) and (37), we can write:

$$\left\{\boldsymbol{\omega}_{k'}\right\} = \left\{\boldsymbol{u}_{k'}^{L}\right\} \begin{bmatrix} \boldsymbol{A} \end{bmatrix}. \tag{39}$$

The variation of the energy of elastic deformation, taking into account (39), will be written in the form:

$$\delta W = \delta \left\{ u_{k}^{L} \right\} \left[A \right] \left[F_{ij}^{k'} \right] \left[H^{ijkl} \right] \left[F_{kl}^{m'} \right]^{I} \left[A \right]^{T} \left\{ u_{m'}^{L} \right\}^{I} + \delta \left\{ u_{k}^{L} \right\} \left[A \right] \left[F_{\theta}^{k'} \right] \left[H^{\theta} \right] \left[F_{\theta}^{m'} \right]^{T} \left[A \right]^{T} \left\{ u_{m'}^{L} \right\}^{T}, \quad (40)$$

or we can write:

$$\delta W = \delta \left\{ u_{k}^{L} \right\} \left[A \right] \left(\begin{bmatrix} F_{ij}^{k} \end{bmatrix} \begin{bmatrix} H^{ijkl} \end{bmatrix} \begin{bmatrix} F_{kl}^{m'} \end{bmatrix}^{T} + \left[F_{\theta}^{k'} \end{bmatrix} \begin{bmatrix} H^{\theta} \end{bmatrix} \begin{bmatrix} F_{\theta}^{m'} \end{bmatrix}^{T} + \left[A \end{bmatrix}^{T} \left\{ u_{m'}^{L} \right\}^{T}.$$
(41)

In the last ratio, the stiffness matrix of the finite element based on the moment scheme for a granular composite material with a dimension of 24×24 will have the form:

$$\begin{bmatrix} K^{k^{\prime}m^{\prime}} \end{bmatrix} = \begin{bmatrix} A \end{bmatrix} \left(\begin{bmatrix} F_{ij}^{k^{\prime}} \end{bmatrix} \begin{bmatrix} H^{ijkl} \end{bmatrix} \begin{bmatrix} F_{kl}^{m^{\prime}} \end{bmatrix}^{T} + \begin{bmatrix} F_{0}^{k^{\prime}} \end{bmatrix} \begin{bmatrix} H^{0} \end{bmatrix} \begin{bmatrix} F_{0}^{m^{\prime}} \end{bmatrix}^{T} \right) \begin{bmatrix} A \end{bmatrix}^{T} .$$
(42)

The global stiffness matrix for the entire body under study is formed based on (2) by summation over all finite elements.

Numerical results. Using the finite element method is virtually impossible without creating software. To implement the presented stiffness matrix of the finite element based on the moment scheme, we will use the "MIPEJIA+" software complex [11], in which we will use the existing preprocessor and postprocessor, and to the preprocessor we will add program blocks that implement the formation of the stiffness matrix described above. To verify the presented mathematical calculations and software implementation, we will determine the stress-strain state of composite structures.

Let us consider the solution of the planar problem of the theory of elasticity for a thick-walled long cylinder under the action of internal and external forces. For an isotropic (quasi-isotropic) material, we will have the following solution:

$$u_r = Ar + \frac{B}{r}.$$
 (43)

We determine the unknown constants A and B from the specified boundary conditions (($\sigma_r(r_1) = -q$), $\sigma_r(r_2) = 0$, where r_1, r_2 – the inner and outer radius of the cylinder, q – the internal pressure, and there is no external pressure). As a result, we have:

$$A = \frac{1 - \nu}{E} \left(\frac{qr_1^2}{r_2^2 - r_1^2} \right), \quad B = \frac{1 + \nu}{E} \left(\frac{qr_1^2r_2^2}{r_2^2 - r_1^2} \right).$$

The material of the matrix is steel with mechanical characteristics of $E^* = 215,8$ GPa; $v^* = 0,3$. The fiber material is tungsten carbide with mechanical characteristics of $E^\circ = 697, 6$ GPa; $v^\circ = 0,3$. The inner radius of the cylinder is $r_1 = 0,1$ m, the outer radius of the cylinder is $r_2 = 0,15$ m, the inner pressure is q = 10 MPa.

The results of calculations with different meshes of finite elements show stable convergence to the analytical solution. Analytical solutions and numerical results for a $6 \times 14 \times 3$ discretization grid are given in Tables 1, 2, 3.

To estimate the error of numerical calculations, we will use the formula:

$$\varepsilon = \frac{\left(u_n - u_a\right)}{u_a} 100\%,$$

where u_a is the analytical solution and u_n is the numerical calculation.

Table 1 shows numerical results for a small volume content of spherical inclusions (f = 0...0,3) and, therefore, elastic constants were calculated according to formulas (5), (6); Table 2 shows the calculations for a large volume content of spherical inclusions (f = 0, 7...1) and, therefore, elastic constants were calculated according to formulas (7), (8). As can be noted, when the volume fraction of a stiffer inclusion increases, the composite material also becomes stiffer and, consequently, the displacements of the points of the inner surface decrease. With the given finite element grid, the maximum error in all cases is about 5%, which is most likely related to errors in the approximation of the geometry of the cylindrical surfaces. The same picture is observed in the case of reinforcement with lamellar inclusions (Table 3), when the elastic characteristics are calculated according to formulas (9), (10).

1	able 1
Displacement of the inner point of the cylin	nder
(spherical inclusions, small volume fracti	on)

Volume content of fiber, <i>f</i>	Analytical solution (formula (43)), ×10 ⁵ m	Numerical solution, MFES, ×10 ⁵ m	Error, %
0	1,344	1,276	-5,06
0,1	1,214	1,154	-4,94
0,2	1,107	1,053	-4,88
0,3	1,017	0,968	-4,82

Table 2Displacement of the inner point of the cylinder(spherical inclusions, large volume fraction)

Volume content of fiber, <i>f</i>	Analytical solution (formula (43)), ×10 ⁵ m	Numerical solution, MFES, ×10 ⁵ m	Error, %
0,7	0,720	0,679	-5,69
0,8	0,580	0,550	-5,17
0,9	0,485	0,461	-4,95
1	0,416	0,395	-5,05

Table 3

Displacement of the inner point of the cylinder (lamellar inclusions, small volume fraction)

Volume content of fiber, f	Analytical solution (formula (43)), ×10 ⁵ m	Numerical solution, MFES, ×10 ⁵ m	Error, %
0	1,344	1,276	-5,06
0,1	1,170	1,113	-4,87
0,2	1,037	0,987	-4,82
0,3	0,930	0,886	-4,73
0,4	0,844	0,804	-4,74
0,5	0,772	0,736	-4,66
0,6	0,712	0,679	-4,63

In the process of calculations, all components of the stress-strain state were obtained, so, in Fig. 2 it is shown the distribution in the cylinder of stress σ_{xx} (the axes are shown in the figure) for a composite with lamellar inclusions (f = 0,2).



Fig. 2. Stress distribution σ_{xx} in a hollow cylinder made of composite material with lamellar inclusions (f = 0,2)

Ľ.×

Conclusions. An approach to numerical modeling of composite structures with discrete inclusions based on homogenization of heterogeneous material is presented. The stiffness matrix of the spatial finite element is constructed on the basis of the moment scheme, which allows calculating composite materials with both compressible and weakly compressible components. Numerical calculations using the developed matrix showed a good convergence of the obtained results to the known exact solutions.

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