Finite element modeling of elastic moduli and microstresses in textile carbon-carbon composites

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Abstracts. The problem of detailed calculation of micro-stresses in textile composite materials under arbitrary types of loading is considered. A model for calculating the effective characteristics of textile composites considering the real complex curvilinear anisotropy of fibers in tissues is proposed. The model is based on the asymptotic homogenization method, whereby local problems of elasticity theory for a curvilinear anisotropic body are formulated. For the numerical solution of these problems, the finite element method is used. The implementation of the proposed method was carried out within the framework of the SMCM software package, developed at the Department of Computational Mathematics and Mathematical Physics of the Bauman Moscow State Technical University. The SMCM software package allows you to perform a full cycle of finite element modeling, including the stages of pre-processing and post-processing. An example of numerical modeling of a textile carbon-carbon composite of twill weaving is carried out. It is shown that the developed software package provides a very high accuracy of calculations of the effective elastic properties of composites. The comparison was carried out with the calculations obtained using the ANSYS software, which was modified to provide the possibility of solving local problems, the relative deviation in the calculations of the effective elastic constants did not exceed (-7) degrees.

Keywords: carbon-carbon composites, textile composites, elastic modules, micro-stresses, modeling, on the method of asymptotic homogenization, the finite element method, software complex

1. Introduction

The possibility of designing composites with specified properties is one of the main tasks to be solved by the efforts of developers of composite materials. This problem is especially urgent for carbon-carbon composites (CCCM) intended for operation in extreme conditions [1-4]. However, in order to solve this problem, it is necessary to have sufficiently accurate methods for calculating the properties of composites, considering the detailed microstructure of composites, and the features of their mechanical properties, such as, for example, the curvilinear anisotropy of monofibers in textiles, which are used as a reinforcing component of the composite. Despite the fact that there are a lot of methods for calculating composites, including finite element methods that consider the micro-structure of composites, the problem of correctly considering the change in the mechanical properties of reinforcing fibers depending on their curvature in the textile is still relevant. Currently existing commercial software packages do not have such functionality. Relatively recently, in the Comsol software package, opportunities have appeared for considering the locally curvilinear anisotropy of thermal conductivity. In [5-12], a method for calculating the effective properties of composites with complex structures based on the finite element solution of local problems over the periodicity cell was proposed. The purpose of this work is to further develop this method with the possibility of automated accounting for the curvilinear-anisotropic properties of reinforcing fibers of composites, and the development of software for automated calculations of micro-stresses in composites, as well as effective elastic characteristics of textile composites.
2. Local problems over periodicity cells

According to the general idea of the homogenization method [8, 10, 13], composites are considered as periodic structures consisting of periodicity cells (PS). Let us further assume that the PS of the composite $V_\xi$ has a geometric symmetry of the arrangement of the composite components (regions $V_{\xi\alpha}$) relative to 3 coordinate planes ($\xi = 0$), where $\xi$ – the local coordinates for one PS. In addition, we assume that there is also physical symmetry, i.e., geometrically symmetric components also have the same elastic characteristics. Then, according to [8, 10], one can consider a set of so-called local problems $L_{pq}$ of the elasticity theory per 1/8 of the composite periodicity cell (PS) $\tilde{V}_\xi$.

Here and below, the contact surfaces $\tilde{\Sigma}_{\xi\alpha\beta}$ of the components inside are denoted as $\tilde{V}_\xi$, $\Sigma_\xi = \{\xi_\xi = 0\}$ – coordinate planes of the PS, $\Sigma_x = \{\xi_x = a_x / 2\}$ – end surfaces of the periodicity cell, $a_x$ – lengths of the PS edges, $s=1,2,3$. Dimensionless local coordinates $\xi_j$ are introduced into the PS, $\sigma_{i(pq)j}$ – micro-stresses, $\varepsilon_{ik(pq)}$ – micro-deformations, $U_{i(pq)}$ – displacements in the $L_{pq}$ problem, the index $\alpha$ indicates the number of the component in the PS (fibers or matrix). For a unidirectional composite, $N=2$. Symbols $U_{i(pq)j}$ mean derivatives with respect to local coordinates $\xi_j$.

Ideal contact conditions are specified on the contact surface of the composite components.

Boundary conditions in $L_{pp}$ problems.

A) On the faces $\Sigma_p = \{\xi_p = 0.5\}$ of 1/8 of the PS, longitudinal displacements and zero tangential components of the stress vector are specified:

$$U_{i(pp)} = (1/2)\tilde{U}_{i(p)}$$

$$S_{i(p(p))} = 0, \quad S_{j(p(p))} = 0$$

(2)

$p = 1,2,3$, $i \neq j \neq p$, $i, j = 1,2,3$

with $S_{ik(pq)} = \sigma_{ik(pq)} n_k$ – tangential components of the stress vector $\sigma_{ik(pq)} n_k$ on the faces $\Sigma_k$.

Б) On the faces $\Sigma_p = \{\xi_p = 0\}$, the sliding conditions are specified
\[ U_{p(pp)} = 0, \quad S_{p(pp)} = 0, \quad S_{pp} = 0 \]  
\( (3) \)

On the remaining faces of \( 1/8 \) of the PS, sliding conditions are specified as well. The value \( \overline{e}_{pp} \) represents given average deformation of the PS.

**Boundary conditions in \( L_{pq} \) problems ( \( p \neq q \)).**

On the faces \( \Sigma_{p} \) and \( \Sigma_{p} \), following boundary conditions are specified:

\[ U_{i(pq)} = 0, \quad S_{pp(pq)} = 0, \quad U_{q(pq)} = 0, \]  
\( (4) \)

\[ p = 1, 2, 3, \quad i \neq q \neq p \neq i, \quad i, p, q = 1, 2, 3 \]

Similar boundary conditions are specified on the faces \( \Sigma_{i} \) and \( \Sigma_{j} \).

On the faces \( \Sigma_{q} \):

\[ U_{q(pq)} = \frac{1}{4} \overline{e}_{pq}, \quad S_{qq(pq)} = 0, \quad U_{i(pq)} = 0, \]  
\( (5) \)

On the faces \( \Sigma_{q} \):

\[ U_{q(pq)} = 0, \quad S_{qq(pq)} = 0, \quad U_{i(pq)} = 0 \]  
\( (6) \)

**Accounting curved fibers anisotropy.**

The fibers in the textile have curvilinear anisotropy [14,15], which is introduced as follows: for each fiber, its own coordinate system \( O_{\xi}^{\alpha} \) connected with a single local coordinate system of the PS using the rotation matrix \( Q^{m(\alpha)}_{\xi} (\xi) \) around the axis, \( \alpha = 1, 2 \), is introduced. The rotation matrix \( Q^{m(\alpha)}_{\xi} (\xi) \) depends on the coordinates \( \xi \). It is assumed that at each point of the PS with coordinates \( O_{\xi} \) the thread can be considered as a 1D composite with effective characteristics that coincide with the corresponding effective characteristics \( C^{m(\alpha)}_{ijkl} \).

In order to find the components of the elasticity moduli tensor of fibers in a single local coordinate system, we use the formulas for transforming the components of the 4th rank tensor when the coordinate system is rotated [15]:

\[ C^{(\alpha)}_{ijkl}(\xi) = \overline{C}^{(d)}_{ijkl} O^{m(\alpha)}_{\xi} (\xi) Q^{n(\alpha)}_{\xi} (\xi) Q^{s(\alpha)}_{\xi} (\xi) Q^{r(\alpha)}_{\xi} (\xi), \]  
\( (7) \)

The matrix of the textile composite is assumed to be isotropic; its of elastic moduli tensor \( C^{(\alpha)}_{ijkl} \) does not depend on the rotation matrix and coordinates:

Further \( L_{pq} \) problems with tensors (7) are solved for a 3-component composite, the PS of which consists of 2 systems of threads and a matrix.
Calculation of effective characteristics. After solving these $L_{pq}$ problems and calculating the micro-stress fields $\sigma_{ij}^{\alpha}$, the values of the effective elastic moduli tensor of the textile composite are calculated

$$C_{ijpq} = \frac{\overline{\sigma}_{ij(pq)}}{\varepsilon_{pq}},$$

$$\overline{\sigma}_{ij(pq)} = \left\langle \sigma_{ij}^{\alpha} \right\rangle = \sum_{\alpha=1}^{N} \int_{\sigma^{\alpha}} \sigma_{ij}^{\alpha} dV$$

Next, the effective elastic compliance tensor $\Pi_{ijpq} = (C_{ijpq})^{-1}$ and the effective elastic characteristics of the composite, which is an orthotropic material, are calculated:

$$E_{\alpha} = \frac{1}{\Pi_{a\alpha\alpha\alpha}}, \quad v_{a\beta} = -\frac{E_{\alpha}}{\Pi_{aa\alpha\beta}}, \quad G_{a\beta} = C_{a\beta}$$

- effective longitudinal and transverse elastic moduli, effective Poisson's ratios and effective interlayer shear moduli.

Numerical modeling results.

Results of numerical modeling of elastic properties of fabric composites in the SMCM software package

For the solution of the local $L_{pq}$ problems, the finite element method (FEM) was used. Details of the numerical FEM algorithm for solving local problems are presented in [12]. The numerical implementation of the developed algorithm, including the implementation of the FEM, was carried out in the SMCM software package developed at the Scientific and Educational Center for Supercomputer Engineering Modeling and Development of Software Systems (SIMPLEX Center) and at the Department of Computational Mathematics and Computational Physics of Bauman State technical University (BMSTU) [16].

Parameterized geometry of textile composites with different microstructures: linen, satin and twill, was created in SMCM software package. FE meshes were generated both in SMCM and ANSYS.

Calculations of micro-stress fields $\sigma_{ij(pq)}^{\alpha}$ and deformations were performed both in the developed SMCM and in the ANSYS software packages on approximately the same FE meshes. During the comparative analysis, the ANSYS software module was modified in order to ensure that all the characteristics necessary for solving the $L_{pq}$ problems were obtained. Comparisons were performed only for normal temperatures at which there are no phase transformations. A FE with a quadratic approximation of solutions relative to displacements (10-node FE) was used. For comparative modeling, a FE mesh with a size of 314583 elements was used. 1/8 of the PC has the shape of a plate with a length of 52.052 along the $Ox$ and $Oz$ axes and a thickness of 2.6989 along the $Oz$ axis (dimensionless coordinates).

The length of the major axis of the oval section of the fibers is 8, and that of the minor axis is 1.15. The fiber concentration is 0.5. In the comparative analysis, the following characteristics of the matrix and fibers, corresponding to carbon fibers and carbon matrix, were used:

$$E_f^0 = 190 \text{ GPa}, \quad \nu_f = 0.2, \quad E_m^0 = 20 \text{ GPa}, \quad \nu_m = 0.27$$

(9)
Figures 1-3 show some of the obtained results of calculating the micro-stress fields $\sigma_{ij}^{\alpha pq}$ in the PS for textile CCCM with a twill weaving structure at normal temperature. The results of comparing the micro-stress fields $\sigma_{ij}^{\alpha pq}$ for all the considered $L_{pq}$ problems showed that the developed SMCM software package provides a very high accuracy of micro-stress calculations, the maximum relative deviation in the calculations obtained in the ANSYS and SMCM did not exceed 1.5-2%. Comparison of the micro-stress fields also shows that the SMCM fully reproduces all the features of these fields, with the presence of the same maxima and minima, which can be obtained using the ANSYS for the complex geometric structure of the textile CCCM.

Figure 1. Distribution of longitudinal normal stresses $\sigma_{11}$ in 1/8 of the PS, in the $L_{11}$ problem for CCCM, obtained using ANSYS (a) and using SMCM (b)

Figure 2. Distribution of transverse normal stresses $\sigma_{22}$ in 1/8 of the PS, in the $L_{22}$ problem for CCCM, obtained using ANSYS (a) and using SMCM (b)
The results of calculating the effective elastic constants for textile CCCM with weave threads and with the characteristics of the components (9) are shown in Table 1. These results demonstrate that the SMCM allows calculating the effective characteristics of textile composites with almost 100% accuracy. The deviation in the calculations with the results obtained using the ANSYS is within the limits of machine accuracy and has -7 ... -9 orders of magnitude.

Table 1. Effective elastic constants of the composite obtained using ANSYS and SMCM for CCCM

| №№   | Effective elastic constants for CCCM | ANSYS     | SMCM     | Relative deviation, % |
|-------|-------------------------------------|-----------|----------|------------------------|
| 1     | $E_1$, ГПа                          | 86.289    | 86.289   | 1.34e-08               |
| 2     | $E_2$, ГПа                          | 46.982    | 46.982   | 1.64e-08               |
| 3     | $E_3$, ГПа                          | 86.284    | 86.284   | 1.71e-08               |
| 4     | $\nu_{12}$                          | 0.248     | 0.248    | 2.32e-08               |
| 5     | $\nu_{23}$                          | 0.134     | 0.134    | 4.53e-08               |
| 6     | $\nu_{13}$                          | 0.172     | 0.172    | 2.81e-08               |
| 7     | $G_{13}$, ГПа                       | 30.122    | 30.122   | 9.67e-08               |
| 8     | $G_{23}$, ГПа                       | 16.506    | 16.506   | 2.06e-07               |
| 9     | $G_{12}$, ГПа                       | 16.506    | 16.506   | 1.69e-08               |
3. Conclusions

A model for predicting the elastic properties of textile carbon-carbon composite materials with complex structures is proposed. The model is based on the method of asymptotic homogenization, which is used to formulate local problems of the theory of elasticity for a curvilinear anisotropic body on a periodicity cell. The proposed model is implemented as part of the SMCM software package, developed at the Department of Computational Mathematics and Mathematical Physics of the Bauman Moscow State Technical.

The performed comparative numerical calculations showed that the developed software implementation of the model as part of the SMCM software package, allows one to obtain results of very high accuracy, both for the effective elastic constants of the CCCM and for the fields of (micro-stresses distribution?) in the PS of the composite. The relative deviation from similar results obtained using the ANSYS does not exceed 1.5-2%.

Calculations of elastic constants for a typical CCCM showed that the developed model, and its implementation as part of the SMCM, makes it possible to predict the full set of elastic properties (21 elastic constants) of composites with very high accuracy.

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