Comparative analysis of averaging methods for obtaining composite material elastic characteristics

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Abstract. Composites are widely used as engineering structural materials in different technical areas, given their higher mechanical properties combined with their smaller weight as compared with the “pure” materials. An important characteristic of a composite is a set of its elastic properties. To determine these properties, both experimental methods and mathematical simulation are used. Due to large material costs and time expenditures inherent in each experiment (fabrication of the material and the test sample, performance of the experiment and processing of the results), on the material design stage, as well as when determining the material application area, preference is given to the simulation methods. This paper is focused on the comparative analysis of the available mathematical simulation methods in terms of performance study of the unidirectional fiber-reinforced composite in the plane normal to the fiber orientation. For illustrative purposes, composites with two different kinds of matrix, polymeric and metal, are considered.

1. Introduction

Currently, composite materials are widely used in different technical areas. These materials are of particular importance in the aerospace and rocket applications where the structural items are exposed to concurrent extreme thermal and mechanical stresses. Alongside with the tough requirements to the thermal and thermomechanical characteristics of structural materials, in these industries, the structural weight is also an essential factor. With the use of the composite materials in different industries, it becomes possible to reduce significantly the structural weight, while retaining, or even improving, the thermomechanical properties of the structural item under development [1]. The most common types of the composite material matrix are polymeric and metal ones. For polymeric composites, various thermoplastics, thermosetting materials and elastomeric materials are most frequently used [2]. The typical metal composites are materials based on the aluminum, titanium, copper or nickel matrix [2].

When designing a composite-based structural item, among the most important characteristics to be considered are the elastic properties of the composite. Experimental investigation of the characteristics of nanocomposites, specifically, the components they are composed of, is often pretty resource-consuming, both in terms of the cost and from the viewpoint of the time required for experiment preparation, performance and result processing. Therefore, to investigate the properties of these materials, mathematical simulation methods are mainly used. These methods can be divided into three groups, namely, analytical methods, numerical methods without the use of the finite-element methods (FEM), and FEM-based methods.
Each group has its own advantages and shortcomings. For example, the analytical methods have been thoroughly studied, do not require too much computing capacity, and impose no requirements to the software (SW). However, the considerable disadvantage of these methods is the necessity of making numerous assumptions that are not always consistent with the reality. The numerical methods make it possible to perform computations in the most general formulation of the task, without making any simplifications or assumptions for the target of research and its properties. The main shortcoming of these methods are their high resource requirements. Hence it is reasonable to perform comparative analysis of the results obtained using different mathematical simulation methods.

In this paper, results obtained by using the best known analytical approaches used by Voigt-Reuss [3], Hashin-Shtrikman [3, 4], as well as the self-consistent method [5], the method outlined in [6], are compared with the results obtained by finite-element simulation using the ANSYS software.]

2. Formulation of the problem
The target of the research is an unidirectional fiber-reinforced periodic composite. The main difficulty when investigating the elastic behavior of such a composite is definition of the elastic properties in the plane normal to the reinforcement direction. This paper addresses a two-dimensional domain (the fiber-reinforced composite cross section normal to the reinforcement direction), with the periodic cell shown in Fig. 1.

![Figure 1. Periodic cell of the region. The materials of the matrix and the inclusion are assumed to be isotropic.](image)

3. Description of the methods. Main relationships
One of the most common and simple approaches to describing the elastic behavior of a composite is the Voigt-Reuss approach that provides the upper and lower estimates for the possible values of the material elastic moduli.

The upper estimate can be obtained by averaging the stresses in the inhomogeneous linearly elastic isotropic medium, assuming its strain state homogeneity. This hypothesis was made by V. Voigt in 1910. The lower estimate can be determined by averaging the deformations in the inhomogeneous linearly elastic isotropic medium, assuming its stress homogeneity. This hypothesis was made by A. Reuss in 1929.

For bulk elasticity modulus $K$ and shear modulus $G$ of a two-component isotropic composite, the Voigt-Reuss model takes the following form:

$$
K_+ = 1 - C_V + C_V \frac{K_i}{K_m},
G_+ = 1 - C_V + C_V \frac{G_i}{G_m},
$$

$$
K_- = \left(1 - C_V + C_V \frac{K_m}{K_i}\right)^{-1},
G_- = \left(1 - C_V + C_V \frac{G_m}{G_i}\right)^{-1}.
$$

(1)

Here $C_V$ – volume concentration of inclusions, $K_-$, $K_i$, $K_m$, $G_i$, $G_m$ – upper and lower estimates of the bulk elasticity modulus and the shear modulus, correspondingly, of the composite according to the Voigt-Reuss method, $K_-$, $K_+$, $G_-$, $G_+$ – bulk elasticity modulus of and shear modulus of the inclusion and the matrix, respectively.
In this paper, for the convenience of presentation and subsequent analysis, Young's modulus $E$ of the composite, associated with bulk elasticity modulus $K$ and shear modulus $G$ via relation $E = \frac{9KG}{3K + G}$, was chosen.

Another approach to estimating the possible values of the material elasticity moduli is known as the Hashin-Shtrikman method [3, 4]. This approach based on the assumption of inhomogeneity of the stress and strain fields involves two functionals: the minimizable (Lagrange functional) and maximizable (the Castiglano functional) ones that coincide with each other the true distributions of displacements and stresses. The estimates obtained by this method are the optimal ones that can be obtained without taking into account the geometry of the particles of the composite components. For elastic deformation, this approach also has an alternative name, namely, “dual variational formulation of the elasticity problem in an inhomogeneous solid”.

In case of a two-component composite consisting of linearly elastic components, the Hashin-Shtrikman method relations have the following form:

$$
\begin{align*}
\bar{K} &= K_m + \frac{C_V (K_i - K_m)}{1 + (1 - C_V) \mu_m (K_i - K_m)}, \\
\bar{G} &= G_m + \frac{C_V (G_i - G_m)}{1 + (1 - C_V) \mu_m (G_i - G_m)}, \\
\bar{K'} &= K_i + \frac{1 + C_V \alpha_i (K_i - K_m)}{1 + C_V \alpha_i (K_m - K_i)}, \\
\bar{G'} &= G_i + \frac{1 + C_V \beta_i (G_i - G_m)}{1 + C_V \beta_i (G_m - G_i)}.
\end{align*}
$$

(2)

Here $\bar{K}, \bar{K'}, \bar{G}, \bar{G'}$ – upper and lower estimates of the bulk modulus of elasticity and the shear modulus of the composite, correspondingly, according to this approach.

One of the methods taking into account the particle geometry of the composite component is the self-consistency method. It involves consideration of the interaction between a single inhomogeneity element (an inclusion or a particle of the matrix) and the homogeneous isotropic medium featuring the design elastic moduli values. With subsequent averaging of the parameter distribution perturbations in these elements over the composite volume, it is possible to obtain the design relationships for the elastic characteristics of the composite. For the two-dimensional formulation of the problem, it is necessary to consider reinforcement based on infinite circular cylinders.

For the target material, the main relations of this method for modules $K$ and $G$ have the following form:

$$
C_V u_{i1} + (1 - C_V) u_{m1} = 0, \quad C_V u_{i2} + (1 - C_V) u_{m2} = 0.
$$

(3)

Here

$$
\begin{align*}
u_{i1} &= u_i \cdots \nu, \quad u_{i2} = u_i \cdots D, \quad u_{m1} = u_m \cdots \nu, \quad u_{m2} = u_m \cdots D,
\end{align*}
$$

$$
\nu_i = (C_i - C + C \cdots W_j)^+ \cdots (C - C_j), \quad u_m = (C_m - C + C \cdots W)^+ \cdots (C - C_m),
$$

$$
C \cdot W = (3K + 4G) V + 5/3((3K + 4G)/(K + 2G) D),
$$

where $W$ – isotropic Eshelby’s tensor, $C = 3KV + 2GD$, $C_i = 3K_iV + 2G_iD$, $C_m = 3K_mV + 2G_mD$ – tensors of the elasticity coefficients of the composite, inclusion and matrix, respectively, $V$ and $D$ – volumetric and deviator components, respectively, of the unit fourth-rank tensor. Tensor $W_i$ corresponds to square matrix $N$ of the sixth order that involves seven independent elements [5]:

$$
\begin{align*}
N_{11} &= N_{22} = QD_{11} + RD_1, \quad N_{12} = N_{21} = QD_{11}/3 - RD_1, \quad N_{33} = QD_{33} + RD_3, \quad N_{31} = N_{32} = b^2 QD_{11} - RD_3,
N_{13} &= N_{23} = QD_{13} - RD_1, \quad N_{66} = QD_{41}/3 + RD_1, \quad N_{44} = N_{55} = Q(1 + b^2) N_{13}/2 + R(1 - D_1)/2.
\end{align*}
$$

(4)

where
The other elements of this matrix are zero. Here \( Q = \frac{3}{2}(1-\nu) \), \( R = \frac{(1/2 - \nu)}{(1-\nu)} \), \( \nu = \frac{(3K/2 - G)}{(3K + G)} \), and \( b \) is the ratio of the cylinder radius to its length for the case of circular cylinder-based reinforcement. To take into account the assumption about unlimited cylinder length, a support study was carried out to show that where \( b \leq 0.01 \), any variations in the coefficients involved in the matrix \( N \) elements can be neglected (see Fig. 2), therefore, value \( b = 0.01 \) can be deemed adequate for describing an infinitely long circular cylinder.

![Figure 2](image)

**Figure 2.** Dependence of auxiliary coefficients \( D_i \) involved in matrix \( N \) elements on \( b \) values.

For fibrous materials, there is an approach described by A.M. Skudra and F.Ya. Bulavs [6]. This method was developed for reinforced plastics. The composite elastic modulus in the direction transverse to the square-type fiber packing (which corresponds to the problem under consideration) can be determined as follows:

\[
E = \left[ \left(1 - r_i \right) \frac{1}{1 - \nu_m^2} + r_i I \right] E_m, \tag{5}
\]

where

\[
I = \frac{1}{a} \left[ \frac{\pi}{2} - \frac{2a}{\sqrt{a^2 - b^2}} \arctg \frac{a - b}{a + b} \right], \quad a = \frac{1 - \nu_i^2}{E_m}, \quad b = r_i \left[ \frac{1 - \nu_i^2}{E_m} - a \right], \quad r_i = \sqrt{\frac{2\pi}{C_v}}.
\]

Here \( E_m, E_i, n_m, n_i \) – Young's moduli and Poisson's coefficients of the matrix and inclusion, respectively.

For the numerical solution of the problem, the ANSYS finite element software was used. For the selected periodic cell of the composite, the relevant geometric boundary conditions were applied to realize the desired homogeneous uniaxial tension and shear according to the method described in [7]. To analyze the scale effect, simulation was performed for a single, four and nine cells of periodicity of the composite. Processing of the results involved building of a system including the stress and strain vectors, constructing of compliance matrix \( S \) for the composite, and determining of the Young modulus from relation \( E = 1/S_{11} \).

### 4. Analysis of the results

As an example of reinforcement for a composite with a polymer and a metal matrix, elastic parameter values GPa and GPa, respectively, were chosen. As reinforcing inclusions for the matrices, those with elastic parameter values GPa and GPa, respectively, were chosen.

Figures 3 and 4 show the results obtained for the polymer and metal matrices.
In Figures 3 and 4, 1 and 2 – upper and lower estimates obtained with the Voigt-Reuss method, 3 and 4 – upper and lower estimates obtained with the Hashin-Shtrikman method, 5 – estimate obtained with the self-consistency method, 6 – estimate obtained by the Skudra-Bulavs method. In Figure 3, the red dots represent the results obtained by finite element modeling using the ANSYS software for a single periodic cell, the blue dots – those obtained for four periodic cells, while the green ones – for nine periodic cells. In Figure 4, the blue dots represent the results of numerical simulation with four periodic cells.

As can be seen from Figures 3 and 4, with the Voigt-Reuss and Hashin-Shtrikman methods, it is possible to estimate the range of possible elasticity modulus values for the composite.

As a result of comparative analysis of the estimates obtained using analytical and numerical methods, it was found that with the volume fraction of inclusions from 0 to 15-20%, the self-consistency method, as well as the Skudra-Bulavs and Reuss methods, provide results that differ from each other by less than 10%.

It was also found that for the composites whose elastic moduli differ by several orders, the Skudra-Bulavs method show good agreement with the numerical simulation. For other ratios of the elasticity moduli of the composite components, the difference between the values obtained by these methods was more than 15%.

5. Conclusions

The existing methods of mathematical modeling, their application areas and limitations for their applicability were analyzed, as exemplified by an isotropic two-component material corresponding to the isotropy plane of an unidirectional fibrous composite reinforced with fibers of the same diameter. The most widely used analytical approaches to description of the composite elastic properties (the Voigt-Reuss method, the Hashin-Shtrikman model, the self-consistency method, and the Skudra-Bulavs method) were analyzed, and numerical modeling of the elastic behavior of such a material was carried out (using the ANSYS finite element software). Influence of different combinations of composite
components elasticity modulus values was investigated. For this purpose, two cases were considered, namely, where the Young's modulus of the inclusion exceeds the Young's modulus of the matrix by several orders (about 100 times) (which corresponds to reinforcement of a soft matrix, e.g. a polymer one, by hard inclusions), and where the difference in the composite components elasticity moduli does not exceed 10 times (which in turn corresponds to reinforcement of a metal matrix).

For numerical simulation, the optimal number of grid elements was chosen based on test analysis. Furthermore, influence of the scale factor was investigated, and the optimal number of periodic cells was determined.

The results presented in this paper illustrate the applicability limits of the most frequently used analytical methods in comparison with the numerical one, which is especially important when choosing an approach to solving a specific application task.

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