Generation of representative volume elements of heterogeneous materials with distributed orientations of inclusions

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Abstract

The work presents the research on the development of computational method that allow to improve a computational efficiency of homogenization of heterogenous materials with distributed orientation of the inclusions. Original contribution of this work is the formulation of novel method of generation of three-dimensional geometry of the representative volume element (RVE) with consideration of the prescribed orientation distribution of the inclusions. The task of a new method is a determination of spatial orientation of the inclusions in such a way that a set of the inclusions represents the prescribed orientation distribution. Proposed method is based on solution of the optimization problem that is formulated as the minimization of the relative difference between given components of fourth order orientation tensor (input data) and components of fourth order orientation tensor that are determined during the computations with respect to accounted variables. An effectiveness of proposed method has been presented by generation of the RVE representing exemplary composite material.

Keywords: representative volume element, distributed orientation, homogenization

1. Introduction

The work presents the research on the development of computational method that allow to improve a computational efficiency of homogenization of heterogenous materials with distributed orientation of the inclusions. The direct homogenization based on finite element analysis of the representative volume element (RVE) is one of the most popular homogenization methods due to its numerous advantages. On the other hand, it requires high computational cost connected with the solution of boundary value problem and with the creation of the inclusions geometry and finite element mesh. Consideration of the distributed orientation of the inclusions typically requires creation of complex RVE containing several hundreds of inclusions [1, 2]. This fact makes the homogenization very time consuming. The paper presents a novel method of generation of the RVE geometry, based on solution of the optimization problem, that allows to represent the prescribed orientation distribution by applying the reduced number of inclusions in comparison with other methods presented in literature. Proposed approach is based on modification of the optimal pseudo-grain discretization method recently formulated by the authors [3].

2. Orientation distribution description

The orientation of unidirectional material is defined by vector p that depends on two spherical angles θ and φ (Fig.1) as follows:

$$p = \left[\cos\theta, \sin\theta\sin\varphi, \sin\theta\cos\varphi\right]^T . \quad (1)$$

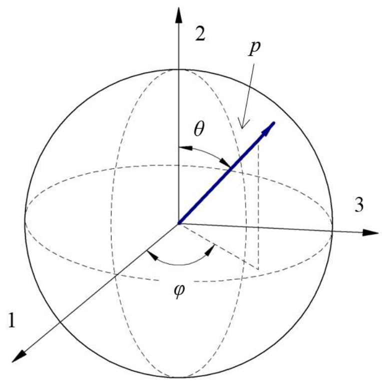

Figure 1: Orientation of single inclusion in terms of spherical angles θ and φ

The orientation distribution function is defined such that the probability of finding an inclusion whose orientation is between p and $(p+dp)$ is $\psi(p)dp$. Usage of orientation distribution function description is cumbersome therefore alternatively the orientation tensor approach of Advani and Tucker [4] has been introduced. Orientation tensors are defined from the dyadic products of the unit vector p and the distribution function $\psi(p)$ over the unit sphere as:

$$a_{ij} = \oint p_i p_j \psi(p) dp, \quad (2)$$

$$a_{ijkl} = \oint p_i p_j p_k p_l \psi(p) dp, \quad (3)$$

$$a_{ij\ldots} = \oint p_i p_j \ldots \psi(p) dp. \quad (4)$$

This work is limited to usage of second and fourth order tensors a_{ij} and a_{ijkl} that are sufficient for the stiffness predictions [4].

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3. Procedure of RVE geometry generation

The task of a new method of the RVE generation is a determination of a spatial orientation of the inclusions in such a way that a set of the inclusions represents the prescribed orientation distribution. The scheme of the proposed approach is presented in the Fig. 2. Input data to the analysis are fourth order orientation tensor describing orientation distribution and geometry of the inclusions. Next step is solution of the optimization problem that allows to find a set of θ and φ angles defining orientation of the inclusions. The optimization problem is formulated as the minimization of the relative difference between given components of fourth order orientation tensor and components of fourth order orientation tensor that are determined during the computations with respect to accounted variables. In order to solve the optimization problem evolutionary algorithm has been applied. To achieve the final result, inclusions with assigned θ and φ angles are placed in the matrix by using random sequential adsorption algorithm (RSA) [2] in a way that prevents from contact between the inclusions. In case of usage of RSA algorithm Digimat software was applied [5].

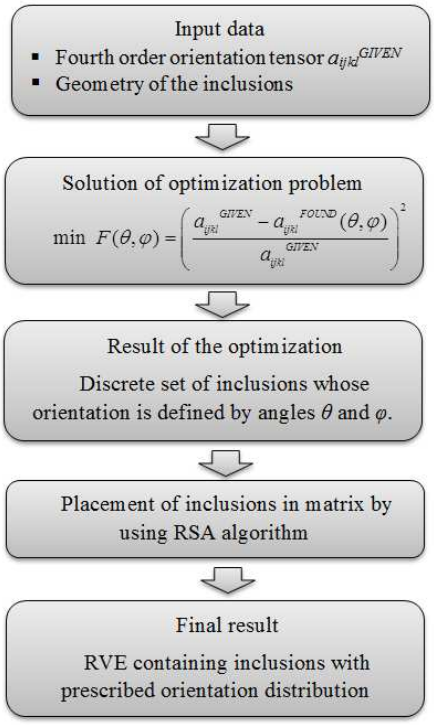

Figure 2: Scheme of proposed method of the RVE generation

The described procedure can deal with any shape and orientation distribution of the inclusions however it has been applied to generate the exemplary RVE containing ellipsoidal particles distributed in accordance with the following fourth order orientation tensor:

$$a_{ijkl}=\begin{bmatrix} 0.5976 & 0.0663 & 0.0383 & 0.0374 & 0.0814 & 0.0513 \\ 0.0663 & 0.1055 & 0.0336 & 0.0559 & 0.0112 & 0.0109 \\ 0.0383 & 0.0336 & 0.0206 & 0.0179 & 0.0151 & 0.0077 \\ 0.0374 & 0.0559 & 0.0179 & 0.0336 & 0.0077 & 0.0112 \\ 0.0814 & 0.0112 & 0.0151 & 0.0077 & 0.0383 & 0.0374 \\ 0.0513 & 0.0109 & 0.0077 & 0.0112 & 0.0374 & 0.0663 \end{bmatrix}. \quad (5)$$

Geometry of the generated RVE containing 30 inclusions is presented in the Fig. 3.

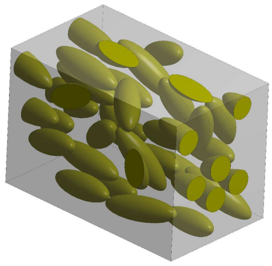

Figure 3: Generated RVE representing the material with prescribed orientation distribution of the ellipsoidal inclusions

The fourth order orientation tensor reconstructed by accounting the inclusions included in the created RVE has the following form:

$$a_{ijkl}=\begin{bmatrix} 0.5977 & 0.0668 & 0.0386 & 0.0371 & 0.0808 & 0.0517 \\ 0.0668 & 0.1045 & 0.0332 & 0.0564 & 0.0113 & 0.0109 \\ 0.0386 & 0.0332 & 0.0204 & 0.0181 & 0.0152 & 0.0076 \\ 0.0371 & 0.0564 & 0.0181 & 0.0332 & 0.0076 & 0.0113 \\ 0.0808 & 0.0113 & 0.0152 & 0.0076 & 0.0386 & 0.0371 \\ 0.0517 & 0.0109 & 0.0076 & 0.0113 & 0.0371 & 0.0668 \end{bmatrix}. \quad (6)$$

4. Conclusions

In conclusion, the number of 30 inclusions was sufficient to represent the prescribed orientation distribution in such a way that relative difference between the components of given fourth order orientation tensor and the components of fourth order orientation tensor reconstructed form the inclusions included in the generated RVE is less than 1%, whereas method presented in the work of Lee et al. [1] required to apply 650 inclusions to obtain similar level of accuracy. The presented approach can lead to significant increase of computational efficiency of the finite element based homogenization of composites with distributed orientations of the inclusions.

In the further work the direct finite element method based homogenization will be performed on the basis of the generated RVE to investigate the mechanical material response. Moreover, materials with different orientation distributions and inclusions shapes will be tested.

References

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