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Generation of the representative volume elements of composite materials with misaligned inclusions

Witold Ogierman*, Grzegorz Kokot

Institute of Computational Mechanics and Engineering, Silesian University of Technology, ul. Konarskiego 18A, 44-100 Gliwice, Poland

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ABSTRACT

The paper presents the novel method of generation of the representative volume elements of composite materials with misaligned inclusions. The novel method, that is based on the solution of the optimization problem, allows to represent the prescribed orientation distribution by applying a reduced number of inclusions, in compariswwwwwon with other methods presented in the literature. The accuracy of the proposed method is demonstrated by the analysis of exemplary orientation distributions. Both the orientation state reconstruction accuracy and the effective material properties prediction accuracy are investigated. Moreover, the effective material properties determined on the basis of the representative volume elements with a reduced number of inclusions are compared with the results of the analysis of representative volume elements containing a large number of inclusions.

1. Introduction

Orientation of the inclusions is one of the primary factors that influences the effective material behavior of a composite. Composite materials with discontinuous reinforcement often reveal anisotropic properties due to distributed orientation of fibers or non-spherical particles. Misaligned inclusions are common in the case of polymer matrix composites reinforced with short fibers manufactured by injection molding [1,2]. Anisotropy caused by distributed orientation of inclusions is also reported in the case of metal matrix composites with ceramic reinforcement [3,4]. Another examples are sisal fiber reinforced composites [5], carbon nanotubes reinforced composites [6] and steel fiber reinforced concrete [7,8]. Due to the increasing popularity of such materials numerical methods that allow to analyze complex spatial orientation of the reinforcement have been developed and discussed in the literature. One of the most popular methods of estimation of the effective properties of materials with distributed inclusions is orientation averaging [9]. In this case effective properties of the material are taken as the weighted average of unidirectional material properties with respect to orientation distribution of inclusions. Advani and Tucker [9] presented expressions that allow to determine the elastic stiffness tensor of a composite with misaligned inclusions in terms of the orientation tensors and the stiffness tensor of a unidirectional composite. In the case of the analysis of nonlinear constitutive behavior the situation is becoming more complicated and consequently homogenization has to be performed in two steps [10–12]. The two-step procedure requires decomposition of the RVE into the so-called pseudo-grains in accordance with the orientation distribution function. Recently, the amount of pseudo-grains required to reconstruct the given orientation distribution has been reduced by developing the optimal pseudo-grain discretization method [13]. The two-step homogenization approach is the most frequently used in the framework of mean field homogenization methods like incremental Mori-Tanaka method [14–16]. The major advantage of a two-step homogenization involving Mori-Tanaka scheme is low computational cost. On the other hand, it usually cannot take into account clustering, percolation, size effects and complex shapes of inclusions. The mentioned limitations may be overcome, for example, by using another widely used homogenization approach that is based on direct finite element (FE) analysis of the representative volume element (RVE) [17–21]. However, in this case, many works report that in order to represent the prescribed orientation distribution accurately a substantial number of inclusions is required. Li et al. [22] investigated the influence of a number of fibers in the RVE on the accuracy of the reconstruction of a given fiber orientation distribution. They concluded that to achieve a satisfactory level of orientation state reconstruction accuracy at least 512 inclusions must be taken into account. Lee et al. [23] who determined the elastic stiffness constants of material reinforced with randomly oriented short fibers reported that achieving reasonable isotropic mechanical properties requires the use of the RVE with 320 inclusions. The RVE representing random orientation of short fibers generated by Tian et al. [24] similarly contains a substantial number of inclusions. On the other hand,

* Corresponding author.
E-mail address: witold.ogierman@polsl.pl (W. Ogierman).

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Böhm et al. [25], to represent a random orientation of the reinforcement phase used a relatively small number of 15 inclusions. They compared the responses of unit cells to loads acting in different directions and reported that differences in the Young's moduli predictions are approximately 4–5%.

The finite element computations performed on the basis of the RVE containing several hundreds of inclusions is very time consuming, especially in nonlinear regime. Therefore, this paper introduces a novel method of RVE generation based on the solution of the optimization problem. In the proposed method, an optimal selection of inclusion orientations reduces the required number of inclusions with no loss of precision in the case of orientation reconstruction.

The paper has the following outline. Section 2 presents general expressions connected with the description of orientation distribution. Section 3 contains details of novel procedure of RVE generation. Section 4 is devoted to the verification of the proposed method by comparing the obtained results with results presented in the literature. Additionally, the results of selected numerical tests have been reported. Section 5 contains conclusions and final remarks.

2. Distributed orientations

2.1. Orientation state description

The orientation of a single inclusion is defined by vector p which can be described by two spherical angles θ and φ (Fig. 1):

$$p = [\sin\theta\cos\varphi,\ \sin\theta\sin\varphi,\ \cos\theta]^T. \tag{1}$$

The orientation state at a point in space can be described by orientation distribution function $\psi(p)$. Orientation distribution function (ODF) is defined as the probability of finding an inclusion whose orientation is between θ_1 and $(\theta_1 + d\theta)$, and φ_1 and $(\varphi_1 + d\varphi)$ is given by:

$$P(\theta_1 \leqslant \theta \leqslant \theta_1 + d\theta,\ \varphi_1 \leqslant \varphi \leqslant \varphi_1 + d\varphi) = \psi(\theta_1, \varphi_1)\sin\theta_1 d\theta d\varphi = \psi(p)dp. \tag{2}$$

Orientation distribution function satisfies the following physical conditions:

$$\psi(\theta, \varphi) = \psi(\pi-\theta, \pi + \varphi) = \psi(p) = \psi(-p), \tag{3}$$

$$\int_{\theta=0}^{\pi}\int_{\varphi=0}^{2\pi} \psi(\theta, \varphi)\sin\theta d\theta d\varphi = \oint \psi(p)dp = 1. \tag{4}$$

While the usage of orientation distribution function can be cumbersome, the orientation tensor approach of Advani and Tucker [9] represents the orientation distribution function in a concise form. Orientation tensors are defined from the dyadic products of the unit vector

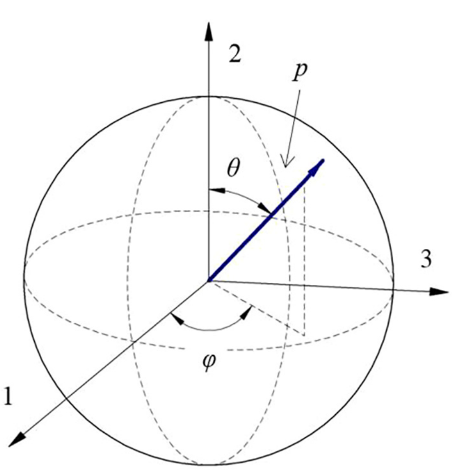

Fig. 1. Orientation tensor p in terms of two spherical angles θ and φ.

p and the distribution function $\psi(p)$ over the unit sphere as:

$$a_{ij} = \oint p_i p_j \psi(p)dp,$$
$$a_{ijkl} = \oint p_i p_j p_k p_l \psi(p)dp,$$
$$a_{ij\ldots} = \oint p_i p_j \ldots \psi(p)dp. \tag{5}$$

There is an infinite number of these tensors in all even orders; however, this work is limited to the usage of the second and fourth order tensors that are sufficient for most uses [9].

2.2. Closure approximation and the reconstruction of the orientation distribution function

In many cases orientation distribution function is unavailable and moreover the only given orientation data is the second order orientation tensor. For example, software dedicated to simulating the injection molding process usually store the second-order tensor a_{ij} only [26]. Therefore, various closure approximations that allow to determine the fourth order orientation from the second order orientation tensor have been developed. One of the most popular is hybrid closure approximation [9]; however, numerous studies report that better accuracy is obtained by using orthotropic or invariant based closures [26–29]. For that reason, during this study, invariant based closure approximation proposed by Chung and Kwon [29] has been considered.

Onat and Leckie [30] proposed the method of reconstruction of orientation distribution function from the second and fourth order orientation tensors. This approach has been successfully used in numerous works [9,12,22]. According to expressions provided by Onat and Leckie [30] ODF can be reconstructed in the following way:

$$\psi(p) \approx \psi_1 + \psi_2 b_{ij} f_{ij}(p) + \psi_3 b_{ijkl} f_{ijkl} \tag{6}$$

where:

$$\psi_1 = \frac{1}{4\pi},\ \psi_2 = \frac{15}{8\pi},\ \psi_3 = \frac{312}{32\pi}, \tag{7}$$

$$b_{ij} = a_{ij} - \frac{1}{3}\delta_{ij}, \tag{8}$$

$$b_{ijkl} = a_{ijkl} - \frac{1}{7}(\delta_{ij}a_{kl} + \delta_{ik}a_{jl} + \delta_{il}a_{jk} + \delta_{jk}a_{il} + \delta_{jl}a_{ik} + \delta_{kl}a_{ij}) + \frac{1}{35}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \tag{9}$$

$$f_{ij} = p_i p_j - \frac{1}{3}\delta_{ij}, \tag{10}$$

$$f_{ijkl} = p_i p_j p_k p_l - \frac{1}{6}(\delta_{ij}p_k p_l + \delta_{ik}p_j p_l + \delta_{il}p_j p_k + \delta_{jk}p_i p_l + \delta_{jl}p_i p_k + \delta_{kl}p_i p_j) + \frac{1}{24}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}). \tag{11}$$

3. Procedure of the RVE generation

A number of strategies for the generation of the representative volume elements of composite materials have been reported in the literature; however, in the case of modeling of misaligned inclusions, the most frequently used approach is based on random sequential adsorption (RSA) [25,31–33] The task of the RVE generation method 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 RVE generation procedure in the framework of RSA method is presented in Fig. 2. The first step is determining the following input parameters: geometry of a single inclusion, volume fraction of inclusions, orientation tensors a_{ij} and a_{ijkl} and the number of inclusions. Then the orientations and positions for new inclusions are created by random processes, a candidate inhomogeneity being accepted if it does not overlap with any of the existing ones and otherwise