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Homogenization of inelastic composites with misaligned inclusions by using the optimal pseudo-grain discretization

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The paper deals with micromechanics of composite materials reinforced with misaligned, non-spherical inclusions. The main goal of this study is focused on numerical treatment of misaligned orientations by using the concept of two-step homogenization. The paper is concerned with the novel method of pseudo-grain discretization based on the optimal selection of pseudo-grains discrete orientations and corresponding weights. In order to solve the optimization problem evolutionary algorithms are used. The proposed approach leads to reduction of the pseudo-grains amount which, in turn, especially in the case of inelastic materials, results in homogenization that is more computationally efficient. The accuracy of the proposed method is presented by analysis of exemplary microstructures. Both the orientation data reconstruction accuracy and stiffness prediction accuracy are discussed. In addition, cases of elastic-plastic material behaviour are analysed and two-step homogenization results are compared with results of direct finite element (FE) based homogenization of representative volume element (RVE) with complex geometry.

1. Introduction

Misaligned orientation of inclusions is common in the case of composite materials reinforced with short fibres or non-spherical particles. The type of materials that are most frequently discussed in the literature are polymer matrix composites reinforced with short fibres manufactured by injection moulding (Advani and Sozer, 2003; Bourmaud et al., 2013; Thi et al., 2015). Other studies of composite with misaligned inclusions are devoted to the analysis of anisotropy of metal matrix composites reinforced with ceramic particles (Jeong et al., 1991; Ganesh and Chawla, 2005). Distributed orientation of the inclusions is also observed in steel fibre reinforced concrete (Wuest et al., 2009; Suuronen et al., 2013). In such cases simplification of orientation distribution and treating it as unidirectional or random can lead to unacceptable errors in predictions of the material behaviour. Therefore, numerical methods that allow to take into account complex spatial orientation of inclusions are introduced and discussed in the literature. One of the most popular methods of estimation of the composite effective properties is direct finite element (FE) analysis of representative volume element (RVE) (Segurado and Llorca, 2002; Pierard et al., 2007; Rassol and Böhm, 2012). Finite element approach can deal with any reinforcement shape and orientation but, on the other hand, it requires high computational cost. Alternatively, boundary element method (BEM) can be applied into homogenization with the main advantages of BEM being high accuracy for materials in complex stress state, easy modification of geometry and reduction of the number of discretizing elements as compared to FEM (Fedeliński et al. 2011; Ptaszny, 2015). The computational effort is connected not only with the solution of boundary value problem, but also with the creation of the inclusions geometry. The generation of spherical or unidirectional oriented inclusions is rather trivial but in the case of misaligned distribution the situation is becoming more complicated. Moreover, finding the geometry that represents accurately prescribed orientation distribution can be cumbersome. Another approach of determining the material effective properties that accounts for misaligned orientations is orientation averaging procedure. 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 (1987) presented explicit expressions that allow to determine elastic stiffness tensor of misaligned composite in terms of orientation tensors and stiffness tensor of unidirectional composite. There are a lot of works that present the effectiveness of this approach for linear material properties (Pierard et al., 2004; Laspalas et al., 2008; Ogierman and Kokot, 2015, 2016). The analysis of nonlinear constitutive behavior is more complex

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and requires orientation distribution function reconstruction and decomposition of the RVE into the so-called pseudo-grains and performing the homogenization in two steps (Lielens et al., 1998). Doghri and Tinel (2005, 2006) presented detailed methodology for two-step homogenization with the use of pseudo-grain discretization procedure. This approach was also applied in multi-scale simulations where FE program is linked at macro-scale to the homogenization procedure at micro-scale (Doghri and Tinel, 2006). The authors of works devoted to two-step homogenization, that were mentioned above, performed the homogenization generally with the use of mean field approaches based on an Eshelby solution (Eshelby, 1957). Kammoun et al. (2011) have extended the two-step homogenization procedure by accounting for a damage phenomenon. Moreover, the procedures proposed by Doghri and Tinel (2005, 2006) is implemented in commercial software Digimat (Adam et al., 2009). Quite similar, but simplified approach based on discrete orientations has been also presented in work of Notta-Cuvier et al. (2013). This paper introduces a novel method of optimal pseudo-grain discretization. In the proposed method, an optimal selection of pseudo-grains orientations and weights can reduce the required amount of pseudo-grains with no loss of precision in the case of orientation reconstruction. From the point of view of computational costs and multi-sale simulations the reduction of pseudo-grain amount is an important issue. During this study description of orientation distribution is expressed by orientation tensors (Advani and Tucker, 1987) and therefore discrete orientation of the pseudo-grains are identified by fitting the fourth order orientation tensor produced by pseudo-grains orientations to fourth order orientation tensor that describes given inclusions orientation distribution.

The paper has the following outline. Section 2 presents general expressions connected with orientation averaging, two-step homogenization and pseudo-grain discretization. In addition, a scheme of RVE decomposition into pseudo-grains as part of the optimization involving evolutionary algorithm is discussed. Section 3 analyses the influence of pseudo-grain discretization on the reconstruction accuracy of orientation tensors. Four different orientations are taken into consideration: exemplary two misaligned orientations, random orientation and orientation analysed by Doghri and Tinel (2006) (in order to compare the results). Section 4 is devoted to the simulation of elastic-plastic material behaviour. The results of two-step homogenization are compared with results of direct FE based homogenization of a representative volume element RVE with complex geometry. Moreover, the behaviour of material with random orientation of inclusions is analysed and the obtained results are compared with the results presented in work of Doghri and Tinel (2006).

2. Homogenization of misaligned composites

2.1. Orientation averaging

In orientation averaging procedure the volume average of any field μ in composite ω is taken as an average of $\mu(p)$ determined for unidirectional composite over all directions weighted by orientation distribution function $\psi(p)$:

$$\langle \mu \rangle_\omega = \oint \mu(p)\psi(p)dp. \tag{1}$$

Unidirectional composite orientation can be defined by vector p which can be described by two spherical angles θ and φ (Fig. 1):

$$p = [\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta]^T. \tag{2}$$

Orientation distribution function is defined as the probability of finding an inclusion whose orientation is between p and $(p+dp)$ is $\psi(p)dp$. Orientation distribution function has the following properties:

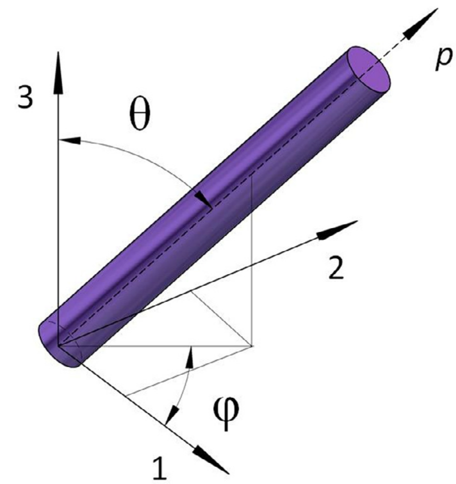

Fig. 1. Orientation vector p in terms of spherical angles θ and φ.

$$\psi(p)dp = \psi(-p)dp, \tag{3}$$

$$\oint \psi(p)dp = 1. \tag{4}$$

While the description of orientation distribution function is cumbersome, the orientation tensor approach of Advani and Tucker (1987) represents the distribution function of fibres in a concise form. Orientation tensors are defined from the dyadic products of the unit vector p and the distribution function $\psi(p)$ over the unit sphere as:

$$a_{ij} = \oint p_i p_j \psi(p)dp, \tag{5}$$

$$a_{ijkl} = \oint p_i p_j p_k p_l \psi(p)dp, \tag{6}$$

$$a_{ij...} = \oint p_i p_j ... \psi(p)dp. \tag{7}$$

There is an infinite number of these tensors in all the even orders but this work is limited to the usage of the second and fourth order tensors that are sufficient for most uses (Advani and Tucker, 1987). Elastic stiffness tensor C_{ijkl} of misaligned composite estimation involving the second and fourth order orientation tensors can be determined by using the following relation:

$$\begin{aligned} C_{ijkl} = {} & B_1 a_{ijkl} + B_2(a_{ij}\delta_{kl} + a_{kl}\delta_{ij}) + B_3(a_{ik}\delta_{jl} + a_{il}\delta_{jk} + a_{jl}\delta_{ik} + a_{jk}\delta_{il}) \\ & + B_4(\delta_{ij}\delta_{kl}) + B_5(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \end{aligned} \tag{8}$$

where B_1–B_5 are scalar constants related to the components of stiffness tensor of unidirectional composite that are presented in detail in work of Advani and Tucker (1987).

2.2. Two-step homogenization

Homogenizing inelastic composite requires the knowledge of orientation distribution function. The orientation distribution function can be recovered from the orientation tensors a_{ij} and a_{ijkl} (Advani and Tucker, 1987; Onat and Leckie, 1988; Doghri and Tinel, 2006). The method that can deal with distributed orientation and nonlinear constitutive behaviour of the inclusions is a two-step homogenization. Misaligned inclusions are divided into groups of unidirectional oriented inclusions characterized by different orientation vectors p. In other words, the RVE is decomposed into a set

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