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Prediction of effective elastic properties of fiber reinforced composites using fiber orientation tensors

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ABSTRACT

The main objective of this work is to give an answer to the question: is it sufficient to consider only the second-order fiber orientation tensor as microstructure variable describing the orientation distribution of short-fiber reinforced composites (SFRCs) in the prediction of effective elastic properties? This question is addressed in the context of SFRCs on the one hand with an overall transversal symmetric orientation distribution of fibers and, hence, effective transversally isotropic properties, and on the other hand with experimentally determined microstructure data using micro-computed tomography. Applying the maximum entropy principle, it is shown, how the fiber orientation distribution function (FODF) can be estimated by relying on the second and/or the fourth-order orientation tensor, only. Both estimates are used within the self-consistent and the interaction direct derivate approach to calculate the effective linear elastic properties. It is shown, that the predicted stiffness tensors significantly depend on the estimation of the FODF. Relative deviations of up to 20% in terms of stiffnesses and up to 46% in terms of Young's modulus are observed. For the experimentally determined microstructure, small deviations of up to 4.3% are found.

1. Introduction

The mechanical properties of composite materials like short-fiber reinforced composites (SFRCs) are crucially dominated by their microstructure. An essential attribute of their microstructure is the orientation distribution of the fibers. The one point statistics of the fiber orientations can be described with fiber orientation distribution functions (FODFs) or, equivalently, with an infinite set of orientation tensors [28]. Kanatani [20] distinguishes three kinds of orientation tensors, which are also called fabric tensors, orientation-moments or order parameters (see, e.g., Gurp [15] and Onat and Leckie [26]).

Second-order orientation tensors frequently appear in literature dealing with composite materials [1,3,4,14,17,18]. Bernasconi et al. [4]; for example, analyzed the fiber orientation distribution of a SFRC using two methods: the first method is based on the observation of the elliptical footprints of the fibers on polished cross sections. The second method starts from a micro-computed tomography (μCT) scan of the material, which then is examined by an image analysis procedure. The results of both methods are compared by means of the second-order orientation tensor.

Second-order orientation tensors are usually the only microstructure related output variable of mold flow simulation packages [13,31]. Dray et al. [14] calculated the thermoelastic properties for an injection molded SFRC. This was done using experimentally determined second and fourth-order orientations tensors, and, additionally, second-order orientation tensors predicted by mold flow simulation. In the latter case, it was necessary to calculate the fourth-order orientation tensor applying closure algorithms. The authors demonstrated the dependence of the thermoelastic properties on the applied closure algorithm (see, e.g., [10]).

Many closure algorithms have been proposed in literature, as, e.g., the linear and the quadratic closure [2], the orthotropic fitted closure [11] and the invariant based optimal fitted closure [10]. The linear and the quadratic closure are directly based on the second-order orientation tensor. The orthotropic fitted closure and the invariant based optimal fitted closure are based on flow data from the calculation of the orientation distribution function. The accuracy of the approximation of the non-fitted closures is only acceptable in particular cases. The fitted closures utilize additional information or assumptions to calculate their predictions.

Further, second-order orientation tensors play a role in the

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homogenization of, e.g., SFRC using full-field approaches. Müller et al. [23] compared predictions of the elastic properties of full-field and mean-field homogenization approaches by means of artificially generated short-fiber microstructure data. The microstructure generation process was based only on the second-order orientation tensor.

Hence, the second-order orientation tensor is commonly used and a well established quantity describing approximately the microstructure of certain composites. However, the question remains open, whether the second-order orientation information is sufficient for the prediction of elastic properties. In the present work, this question is addressed for the special case of transversal symmetric fiber orientation distributions.

The outline of the present paper is as follows: in Section 2, the properties of fiber orientation distribution functions (FODFs) and a classification of different kinds of orientation tensors are described, especially, with a focus on orientation tensors with transversal symmetry. Section 3 deals with the estimation of the FODF based on leading orientation tensors. In Section 4, the theoretical background of the applied homogenization methods, the self-consistent (SC) and the interaction direct derivative (IDD) approach is given. In Section 5, the estimations of the FODFs and the homogenization results are presented for model microstructures and μCT data. Conclusions are given in Section 6.

Notation. A direct tensor notation is preferred throughout the text. If tensor components are used, then Latin indices are used and Einstein's summation convention is applied. Vectors and second-order tensors are denoted by lowercase and uppercase bold letters, e.g., $\boldsymbol{a}$ and $\boldsymbol{A}$, respectively. Additionally, second and higher-order tensors are written as $\boldsymbol{A}_{\langle\alpha\rangle}$, where α indicates the tensor rank. The composition of two second-order or two fourth-order tensors is formulated by $\boldsymbol{AB}$ and $\mathbb{AB}$. A linear mapping of second-order tensors by a fourth-order tensor is written as $\boldsymbol{A} = \mathbb{C}[\boldsymbol{B}]$. The scalar product is denoted by $\boldsymbol{A}\cdot\boldsymbol{B}$. We define the composition operator $\square$ via $(\boldsymbol{A}\square\boldsymbol{B})[\boldsymbol{C}] = \boldsymbol{ACB}$, the dyadic product operator $\otimes$ as $(\boldsymbol{A}\otimes\boldsymbol{B})[\boldsymbol{C}] = (\boldsymbol{B}\cdot\boldsymbol{C})\boldsymbol{A}$, and the contraction operator $[\![\cdot]\!]$ with $(\boldsymbol{a}\otimes\boldsymbol{b})\cdot(\mathbb{C}[\![\boldsymbol{a}\otimes\boldsymbol{b}]\!]) = (\boldsymbol{a}\otimes\boldsymbol{a})\cdot(\mathbb{C}[\boldsymbol{b}\otimes\boldsymbol{b}])$. Higher-order dyadic products of the same tensor are indicated by $\boldsymbol{n}^{\otimes\alpha} = \boldsymbol{n}\otimes\cdots\otimes\boldsymbol{n}$, where $\boldsymbol{n}^{\otimes\alpha}$ is a tensor with the rank α times the rank of $\boldsymbol{n}$. Arbitrary vectors $\boldsymbol{a}$ and $\boldsymbol{b}$, second-order tensors $\boldsymbol{A}$, $\boldsymbol{B}$ and $\boldsymbol{C}$ and the fourth-order tensor $\mathbb{C}$ are used in the foregoing definitions. The identity on symmetric second-order tensors is denoted by $\mathbb{I}^S$. Completely symmetric and traceless, i.e. irreducible tensors are denoted with a prime, e.g., $\boldsymbol{A}'$.

2. Fiber orientation distribution function

2.1. Properties of fiber orientation distribution functions

Throughout this work, the terms "orientation" or "direction" in context of fiber orientations are both describing an axis $\boldsymbol{n}$ of a straight fiber with a constant diameter d and circular profile. The FODF specifies the volume fraction $\mathrm{d}v/v$ of all fibers with a certain orientation $\boldsymbol{n}$ (see, e.g., Zheng and Zou [33]):

$$\frac{\mathrm{d}v}{v}(\boldsymbol{n}) = f(\boldsymbol{n})\,\mathrm{d}S. \tag{1}$$

The quantity $\mathrm{d}S$ is a surface element of the unit sphere $S := \{\boldsymbol{n}\in\mathbb{R}^3 : \|\boldsymbol{n}\| = 1\}$ in the three-dimensional Euclidean space $\mathbb{R}^3$. In spherical coordinates, $\mathrm{d}S = \sin(\vartheta)\,\mathrm{d}\varphi\,\mathrm{d}\vartheta/(4\pi)$ holds with the polar and azimuthal angles ϑ and φ. Generally, an FODF is normalized and non-negative:

$$\int_S f(\boldsymbol{n})\mathrm{d}S = 1, \quad f(\boldsymbol{n}) \geq 0\,\forall\boldsymbol{n}\in S. \tag{2}$$

Since fibers are not truly directional, $f(\boldsymbol{n}) = f(-\boldsymbol{n})$ holds. FODFs with this property are called to be centrosymmetric [33] or antipodal symmetric.

2.2. Empirical fiber orientation distribution function

For a set of N equal weighted fiber orientations $\boldsymbol{n}$, the empirical FODF is defined as

$$f(n) = \frac{1}{N}\sum_{\alpha=1}^{N}\delta(n - n_\alpha). \tag{3}$$

Herein, $\delta(\boldsymbol{n} - \boldsymbol{n}_\alpha)$ is the Dirac delta distribution.

2.3. Orientation tensors

Kanatani [20] distinguished three different kinds of orientation tensors. The orientation tensors of the first kind are moment tensors of the dyadic products of the direction $\boldsymbol{n}$:

$$\boldsymbol{N}_{\langle\beta\rangle} = \int_S f(\boldsymbol{n})\boldsymbol{n}^{\otimes\beta}\mathrm{d}S, \tag{4}$$

whereas, $\boldsymbol{n}^{\otimes\beta}$ specifies a $(\beta-1)$-times tensor product. In case of the empirically defined FODF, the first kind orientation tensors result to

$$\boldsymbol{N}_{\langle\beta\rangle} = \frac{1}{N}\sum_{\alpha=1}^{N}\boldsymbol{n}_\alpha^{\otimes\beta}. \tag{5}$$

Orientation tensors of the first kind are entirely symmetric. Since the FODF is an even function, they are only of even rank. A contraction of a β-order tensor reduces the rank and delivers the orientation tensor $\boldsymbol{N}_{\langle\beta-2\rangle}$:

$$\boldsymbol{N}_{\langle\beta\rangle}[\boldsymbol{I}] = \boldsymbol{N}_{\langle\beta-2\rangle}\ \forall\beta\in\{2,4,6,\ldots\}. \tag{6}$$

Hence, the orientation tensors of the first kind are not linearly independent.

Since the orientation tensors of the second kind do not play a role in this work, the reader is referred to [20] for details. The orientation tensors of the third kind are defined as the entirely symmetric and traceless part of the first-kind orientation tensors:

$$\boldsymbol{D}_{\langle\alpha\rangle} = (\boldsymbol{N}_{\langle\alpha\rangle})'. \tag{7}$$

These tensors are referred to as irreducible tensors. It can be shown, that they are linear independent from each other [20].

2.4. Irreducible orientation tensors of second and fourth-order with transversal symmetry

An irreducible orientation tensor of second-order $\boldsymbol{D}_{\langle 2\rangle}$, which possesses a transversal symmetry with respect to the $\boldsymbol{e}_3$-axis of an orthonormal basis system $\{\boldsymbol{e}_1,\boldsymbol{e}_2,\boldsymbol{e}_3\}$, can be fully described with one independent parameter ξ:

$$\boldsymbol{D}_{\langle 2\rangle} = -\frac{1}{2}\xi(\boldsymbol{e}_1\otimes\boldsymbol{e}_1 + \boldsymbol{e}_2\otimes\boldsymbol{e}_2) + \xi\boldsymbol{e}_3\otimes\boldsymbol{e}_3. \tag{8}$$

An irreducible fourth-order tensor $\boldsymbol{D}_{\langle 4\rangle}$ with a transversal symmetry with respect to the $\boldsymbol{e}_3$-axis can also be fully described with one parameter [8]. Using the normalized Voigt notation, as