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Representation of Hashin–Shtrikman bounds of cubic crystal aggregates in terms of texture coefficients with application in materials design

Thomas Böhlke *, Mauricio Lobos

Chair for Continuum Mechanics, Institute of Engineering Mechanics, Karlsruhe Institute of Technology (KIT), Kaiserstraße 10, 76131 Karlsruhe, Germany

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Abstract

The Hashin–Shtrikman bounds of aggregates of cubic crystals are explicitly represented in terms of tensorial texture coefficients. The formula is valid for arbitrary crystallographic textures and isotropic two-point statistics. The isotropy of the two-point statistics implies that the grain shape is isotropic on average. The new explicit representation has the advantage that the set of energetically admissible crystallographic textures and corresponding effective linear elastic properties can be directly determined and analyzed based on minimum principles of the elastic strain energy density. It is shown that all energetically admissible textures with maximum anisotropy have an effective elastic behavior with cubic sample symmetry. Furthermore, it is proven that there exist texture states without maximum anisotropy which have the extreme elastic properties peculiar to states with maximum anisotropy. This is an important result for the design of elastic material properties.

Keywords: Cubic crystal aggregates; Effective linear elastic properties; Hashin–Shtrikman bounds; Materials design; Tensorial texture coefficients

1. Introduction

The generally non-linear and anisotropic constitutive behavior of polycrystalline metals is dominated by both their microstructure on the grain scale and the properties of the grains. A prominent example is the anisotropic plastic flow behavior of textured metals, which is of utmost importance for the optimization of metal forming operations and the properties of structural parts. Random heterogeneous materials, e.g., polycrystals, can in general be statistically described by n-point probability functions [36]. Many theoretical and numerical studies have shown that one- and two-point probability functions allow for rather accurate predictions of the effective material behavior. The one-point probability function of crystal orientations [11,13] gives a volume fraction description of lattice orientation. In engineering and materials science, this is commonly called the crystalline orientation distribution function (CODF). If the CODF is non-uniform, then the material is said to have a crystallographic texture. Higher-order probability functions describe morphological aspects of the grain structure, e.g., the average grain shape (morphologic texture). The probability functions can be determined experimentally on two- or three-dimensional spatial grids, e.g., by electron backscatter diffraction techniques (see, e.g., [34,16]).

The CODF has been described based on different mathematical formulae [24]. From a continuum mechanical point of view, tensorial representations of the CODF are of advantage since they fit best into the continuum mechanical framework. For an overview of tensorial representations of orientation distributions see [1,21,41,42]. For applications of tensorial representations in the context of homogenization problems see, e.g., [26–28,10].

* Corresponding author.
E-mail addresses: thomas.boehlke@kit.edu (T. Böhlke), mauricio.lobos@kit.edu (M. Lobos).

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In continuum mechanics, n-point probability functions are used to homogenize the effective properties of polycrystals [24,36]. Furthermore, based on homogenization schemes, the effective properties of polycrystals can be optimized by selecting processing paths which induce crystallographic and morphological textures with preferable effective properties [5,19]. In the last decade, important contributions in the context of materials and microstructure design have been made for linear and non-linear constitutive behavior (see, e.g., [2,4,3]).

In this paper we consider the microstructure property linkage in the context of linear elasticity. Based on a new explicit representation of Hashin–Shtrikman bounds for cubic crystal aggregates in terms of a fourth-order tensorial texture coefficient, the effective elastic properties are explicitly represented. The main assumptions for the derivation of the new representation are that (i) the displacement field on the grain scale is continuous, and (ii) the local elastic behavior is linear, uniform and shows a cubic symmetry. Additionally, it is assumed that (iii) the two-point correlation function of grain orientations is isotropic, which implies that the grain geometry is spherical on average. To the best of our knowledge, an explicit representation of the Hashin–Shtrikman bounds in terms of tensorial texture coefficients has not been published yet.

Based on the new representation, the effective elastic properties are discussed in detail. Energetically admissible textures are identified in terms of fourth-order texture coefficients, and corresponding extreme linear elastic properties are derived. With the new approach, it can be shown, for example, that the extreme elastic properties observed at the single crystalline level are transferred completely to effective properties for all textures with a fourth-order texture coefficient on the boundary of the energetically admissible texture range.

The outline of the paper is as follows: in Section 2, the Hashin–Shtrikman bounds are derived in terms of fourth-order texture coefficients. Section 3 gives the energetically admissible fourth-order texture coefficients for different sample symmetries. The implications of first- and second-order bounds on the effective elastic properties are discussed in Section 4, with focus on the transfer of extreme properties from the micro- to the macroscale.

Notation. A direct tensor notation is preferred throughout the text. If tensor components are used, then Latin indices are used and the Einstein's summation convention is applied. Vectors and second-order tensors are denoted by lowercase and uppercase bold letters, e.g. $\boldsymbol{a} \in V$ and $\boldsymbol{A} \in Lin$, respectively. The compositions of two second-order or two fourth-order tensors are 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 and the dyadic product are denoted, for example, by $\boldsymbol{A} \cdot \boldsymbol{B}$ and $\boldsymbol{A} \otimes \boldsymbol{B}$, respectively. We define $(\boldsymbol{A}\square\boldsymbol{B})[\boldsymbol{C}] = \boldsymbol{ACB}\ \forall \boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C} \in Lin$ and $(\boldsymbol{a} \otimes \boldsymbol{b}) \cdot (\mathbb{C}[\![\boldsymbol{a} \otimes \boldsymbol{b}]\!]) = (\boldsymbol{a} \otimes \boldsymbol{a}) \cdot (\mathbb{C}[\boldsymbol{b} \otimes \boldsymbol{b}]) \forall \boldsymbol{a}, \boldsymbol{b} \in V$. The $\bigstar$ denotes the Rayleigh product, which, for tensors of arbitrary rank with respect to an orthonormal basis $\mathbb{T} = T_{ij\ldots l}\, \boldsymbol{e}_i \otimes \boldsymbol{e}_j \otimes \ldots \otimes \boldsymbol{e}_l$, is defined by $\boldsymbol{Q} \bigstar \mathbb{T} = T_{ij\ldots l}(\boldsymbol{Qe}_i) \otimes (\boldsymbol{Qe}_j) \otimes \ldots \otimes (\boldsymbol{Qe}_l)$. The major transposition of $\mathbb{A}$ is denoted by $\mathbb{A}^{\mathsf{T_H}}$, which satisfies $\boldsymbol{A} \cdot (\mathbb{A}[\boldsymbol{B}]) = \boldsymbol{B} \cdot (\mathbb{A}^{\mathsf{T_H}}[\boldsymbol{A}])\ \forall \boldsymbol{A}, \boldsymbol{B} \in Lin$. The identity on symmetric second-order tensors is denoted by $\mathbb{I}^{\mathsf{S}}$. Completely symmetric and traceless tensors are designated by a prime, e.g., $\boldsymbol{A}'$. The brackets $\langle\cdot\rangle$, e.g., $\langle\boldsymbol{\varepsilon}\rangle$, indicate ensemble averaging, which for ergodic media can be identified with volume averages in the infinite volume limit. A superimposed bar, e.g., $\bar{\boldsymbol{\varepsilon}}$, indicates that the quantity refers to the macroscale. The set of proper orthogonal tensors is denoted by $SO(3)$. A short introduction of the tensor calculus used in the present work can be found in [37], as well as in [35].

2. Homogenization of linear elastic properties

2.1. Tensorial representation of the crystallite orientation distribution function

The orientation of a crystal with cubic symmetry is described by a proper orthogonal tensor $\boldsymbol{Q} = \boldsymbol{g}_i \otimes \boldsymbol{e}_i$, where the vectors $\{\boldsymbol{g}_i\}$ and $\{\boldsymbol{e}_i\}$ denote the orthonormal lattice vectors and an arbitrary fixed orthonormal reference basis, respectively. The crystallite orientation distribution function (CODF) $f(\boldsymbol{Q})$ specifies the volume fraction $\mathrm{d}v/v$ of crystals with the orientation $\boldsymbol{Q}$ [11], i.e. $\mathrm{d}v/v(\boldsymbol{Q}) = f(\boldsymbol{Q})\mathrm{d}Q$. Here, $\mathrm{d}Q$ is the volume element in $SO(3)$ which ensures an invariant integration over $SO(3)$ [20]. The probability density function $f(\boldsymbol{Q})$ is non-negative and normalized. It reflects both the symmetry of the crystallites forming the aggregate and the sample symmetry, which results from the processing history [12]. The crystal symmetry implies $f(\boldsymbol{Q}) = f(\boldsymbol{QH}^C) \forall \boldsymbol{H}^C \in S^C \subseteq SO(3)$, where S^C denotes the symmetry group of the crystallite. The sample symmetry requires $f(\boldsymbol{Q}) = f(\boldsymbol{H}^S\boldsymbol{Q}) \forall \boldsymbol{H}^S \in S^S \subseteq SO(3)$. Here, S^S denotes the symmetry group of the sample.

For the analysis in this paper we use a tensorial Fourier expansion of the CODF. For its existence, it has to be assumed that the CODF is square integrable. For the special case of a cubic crystal symmetry, the expansion has the following form [1,21,6,7]:

$$f(\boldsymbol{Q}) = 1 + \sum_{i=1}^{\infty} f_{\alpha_i}(\boldsymbol{Q}), \qquad f_{\alpha_i} = \mathbb{V}'_{\langle\alpha_i\rangle} \cdot \mathbb{F}'_{\langle\alpha_i\rangle}(\boldsymbol{Q}),$$
$$\mathbb{F}'_{\langle\alpha_i\rangle}(\boldsymbol{Q}) = \boldsymbol{Q} \bigstar \mathbb{T}'_{\langle\alpha_i\rangle}, \tag{1}$$

where $\{\alpha_i\} = \{4, 6, 8, 9, 10, \ldots\}$. The $\mathbb{V}'_{\langle\alpha_i\rangle}$ are called tensorial Fourier coefficients, or texture coefficients. The bracket $\langle\cdot\rangle$ in subscript indicates the tensor rank, e.g., $\mathbb{V}'_{\langle 4\rangle}$ is the fourth-order texture coefficient. The tensors $\mathbb{T}'_{\langle\alpha_i\rangle}$ are called reference tensors. They are normalized without loss of generality as follows: $\|\mathbb{T}'_{\langle\alpha_i\rangle}\| = 2\alpha_i + 1$. The $\mathbb{V}'_{\langle\alpha_i\rangle}$ and $\mathbb{T}'_{\langle\alpha_i\rangle}$ are completely symmetric and traceless tensors. For example, the following relations hold for $\mathbb{V}' = \mathbb{V}'_{\langle 4\rangle}$:

$$V'_{ijkl} = V'_{jikl} = V'_{klij} = V'_{kjil} = \ldots, \quad V'_{iikl} = 0. \tag{2}$$