PAMM · Proc. Appl. Math. Mech. **14**, 533 – 534 (2014) / **DOI** 10.1002/pamm.201410254

# Bounds and an isotropically self-consistent singular approximation of the linear elastic properties of cubic crystal aggregates for application in materials design

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For crystal aggregates, the orientation distribution of single crystals affects the anisotropic linear elastic properties. In the singular approximation for cubic materials, this influence is reflected by a fourth-order texture coefficient. From this approximation, the statistical bounds of Voigt, Reuss and Hashin-Shtrikman, and an isotropically self-consistent singular approximation can be obtained. Here, an approximation is called isotropically self-consistent, if, for a vanishing texture, it results in the isotropic self-consistent approximation. The isotropically self-consistent singular approximation has the following advantages: i) it lies between the bounds of Voigt, Reuss and Hashin-Shtrikman, ii) it offers a useful approximation of the effective material behavior of textured anisotropic polycrystals, and iii) it can be used for material design purposes tailoring anisotropic properties mainly depending on the crystallographic texture.



## 1 Introduction

The anisotropic linear elastic behavior of crystal aggregates is influenced by the microstructural information of the polycrystal. The principal microstructural influence considered is the crystallite orientation distribution function (codf), which reflects information of the amount of crystallites having a specific orientation. Based on the Fourier expansion of the codf, the first-order bounds of Voigt and Reuss and the second-order bounds of Hashin-Shtrikman can be derived in terms of the texture coefficients (see, e.g., [2] and [6]). These bounds are related to the singular approximation of [4]. In the present work, an isotropically self-consistent approximation is defined and discussed, based on the results given in [4] and [1].

## 2 The codf and the singular approximation

The stiffness tensor of cubic single crystals is given by its projector representation, see [6],

$$\mathbb{C} = \lambda_1 \mathbb{P}_1^c + \lambda_2 \mathbb{P}_2^c + \lambda_3 \mathbb{P}_3^c \,. \tag{1}$$

In [3], the Fourier expansion of the codf of crystal orientations $\boldsymbol{Q} \in SO(3)$ is introduced in form of

$$f(\boldsymbol{Q}) = 1 + \sum_{i=1}^{\infty} \mathbb{V}'_{\langle\alpha_i\rangle} \cdot (\boldsymbol{Q} \star \mathbb{T}'_{\langle\alpha_i\rangle}) \,, \quad \mathbb{V}'_{\langle\alpha_i\rangle} = \int_{SO(3)} \boldsymbol{Q} \star \mathbb{T}'_{\langle\alpha_i\rangle} f(\boldsymbol{Q}) \, \mathrm{d}Q \,, \quad \|\mathbb{V}'_{\langle\alpha_i\rangle}\| \in [0,1] \,, \tag{2}$$

where the codf is represented by its texture coefficients $\mathbb{V}'_{\langle\alpha_i\rangle}$. The Frobenius norm of the texture coefficients reflects the crystallographic anisotropy of the codf, $\|\mathbb{V}'_{\langle\alpha_i\rangle}\| = 0$ holds for an isotropic codf (vanishing texture), $\|\mathbb{V}'_{\langle\alpha_i\rangle}\| = 1$ for a single crystal orientation. The fourth-order texture coefficient $\mathbb{V}'_{\langle 4\rangle} = \mathbb{V}'$ reflects the influence of the codf on the singular approximation of the stiffness tensor of cubic crystal aggregates [4]

$$\mathbb{C}^{SA} = \left(\lambda_1 \mathbb{P}_1 + \alpha \mathbb{P}_2 + \beta \mathbb{V}'\right) \left(\mathbb{P}_1 + \gamma \mathbb{P}_2 + \eta \mathbb{V}'\right)^{-1} . \tag{3}$$

An isotropic comparison material $\mathbb{C}_0 = c_1 \mathbb{P}_1 + c_2 \mathbb{P}_2$ is used, with $c_1 = \lambda_1$. The functions $\alpha, \beta, \gamma$ and $\eta$ depend solely on the material constants of the cubic material and the eigenvalues of the isotropic comparison material. The tensors $\mathbb{P}_1$ and $\mathbb{P}_2$ denote the identities on spherical and deviatoric second-order tensors, respectively. The singular approximation (3) can be used in order to obtain the first-order bounds of Reuss and Voigt, respectively given in [2] by

$$\mathbb{C}^R = \left(\mathbb{S}^{RI} + \zeta^R \mathbb{V}'\right)^{-1} = \mathbb{C}^{SA}(c_2 \to 0) \,, \qquad \mathbb{C}^V = \mathbb{C}^{VI} + \zeta^V \mathbb{V}' = \mathbb{C}^{SA}(c_2 \to \infty) \,, \tag{4}$$

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with the isotropic tensors $\mathbb{C}^{VI}$ and $\mathbb{S}^{RI}$ and the scalar quantities $\zeta^V$ and $\zeta^R$, which depend only on the material constants of the cubic material. The lower and the upper Hashin-Shtrikman bounds (second-order bounds for isotropic two-point statistics) presented in [6], $\mathbb{C}^{HS-}$ and $\mathbb{C}^{HS+}$, respectively, can be obtained as follows

$$\mathbb{C}^{HS-} = \mathbb{C}^{SA}(c_2 = \min\{\lambda_2, \lambda_3\}) \,, \qquad \mathbb{C}^{HS+} = \mathbb{C}^{SA}(c_2 = \max\{\lambda_2, \lambda_3\}) \,. \tag{5}$$

The first- and second-order bounds enclose the effective material behavior of the polycrystal $\bar{\mathbb{C}}$ as follows

$$\mathbb{C}^{R} \leq \mathbb{C}^{HS-} \leq \bar{\mathbb{C}} \leq \mathbb{C}^{HS+} \leq \mathbb{C}^{V} \,, \tag{6}$$

where the inequalities are to be interpreted as their corresponding bilinear forms on second-order tensors.

Based on the singular approximation (3) of [4], the following approximation is defined by using the isotropic self-consistent solution $c_2^{SC}$ of [1]

$$\mathbb{C}^{ISC} = \mathbb{C}^{SA}(c_2 = c_2^{SC}) \,, \qquad \mathbb{C}^{ISC}(\mathbb{V}' = \mathbb{O}) = \lambda_1 \mathbb{P}_1 + c_2^{SC} \mathbb{P}_2 \,. \tag{7}$$

For vanishing texture (i.e., $\mathbb{V}' = \mathbb{O}$), this approximation results in the isotropic self-consistent approximation and, therefore, it is called isotropically self-consistent. This property makes the approximation (7) a useful anisotropic approximation of the effective anisotropic material behavior of textured polycrystals depending solely on the one-point statistics (the codf).

It should be noted, that the texture coefficient $\mathbb{V}'$ is the only anisotropic tensor in the singular approximation (3). If the texture coefficient is, e.g., orthotropic, so are $\mathbb{C}^{SA}$, $\mathbb{C}^{V,R}$, $\mathbb{C}^{HS\pm}$ and $\mathbb{C}^{ISC}$. This has been shown analogously for the Hashin-Shtrikman bounds (5) in [6], together with admissible domains for the texture coefficient.

## 3 Linear elastic characteristics

Using the bounds of Voigt, Reuss and Hashin-Shtrikman, linear elastic characteristics as Young's modulus can be examined, together with the isotropically self-consistent approximation. The anisotropic Young's modulus of a material with stiffness $\mathbb{C}$ considering the tensile direction $\boldsymbol{n}$ can be defined by the tensorial relation

$$E = \left( (\boldsymbol{n} \otimes \boldsymbol{n}) \cdot \mathbb{C}^{-1} [\boldsymbol{n} \otimes \boldsymbol{n}] \right)^{-1} \,, \tag{8}$$

with fixed tensile direction $\boldsymbol{n}$. This definition conserves the bounds hierarchy (6), see [6]. Young's modulus can be analyzed for polycrystals made of, e.g., copper ($C_{1111} = 168.4\text{GPa}, C_{1122} = 121.4\text{GPa}, C_{2323} = 75.39\text{GPa}, c_2^{SC} = 96.34\text{GPa}$) and arbitrary macroscopic symmetries (induced by adapting solely $\mathbb{V}'$). It can be shown, that there exist states of the codf without a maximum anisotropy ($\|\mathbb{V}'\| < 1$) but with extremal mechanical behavior in some directions, see [6]. In Fig. 1a, Young's modulus of a copper single crystal is depicted. In Fig. 1b, Young's modulus of a polycrystal made of copper with orthotropic macroscopic symmetry shows the maximal value for copper even without a maximum anisotropy of the codf ($\|\mathbb{V}'\| \approx 0.7$). The isotropically self-consistent approximation lies between all bounds.

The first-, second-order bounds and the isotropically self-consistent approximation in terms of texture coefficients can be used for tailoring anisotropic properties for future applications in the field of materials design, as presented, e.g., in [5].

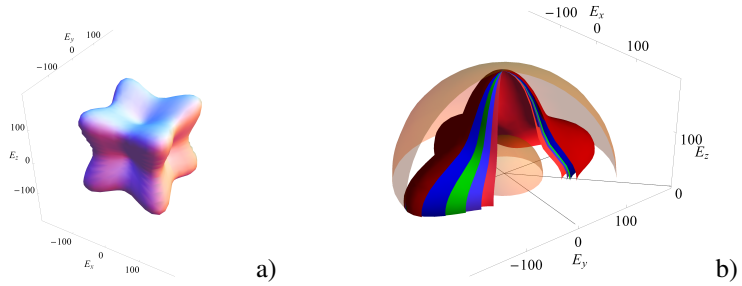


**Fig. 1:** Polar plot of Young's modulus **a** of a copper single crystal and **b** of a polycrystal made of copper with macroscopic orthotropic symmetry without maximum anisotropy for the codf ($\|\mathbb{V}'\| \approx 0.7$) for $\mathbb{C}^{R}$ (light red), $\mathbb{C}^{V}$ (dark red), $\mathbb{C}^{HS-}$ (light blue), $\mathbb{C}^{HS+}$ (dark blue) and $\mathbb{C}^{ISC}$ (green) within the maximum (upper sphere) and minimum (lower sphere) values reachable for copper

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