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Isotropic orientation distributions of cubic crystals

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Abstract

The determination of the effective elastic properties of aggregates of crystalline grains with or without texture is a long standing problem. Presently, such averages are investigated and their anisotropy is quantified by an anisotropy tensor. The harmonic decomposition of fourth-order tensors is applied to both the elasticity tensors of single crystals with cubic symmetry as well as to the effective elasticity tensors of aggregates of cubic single crystals. It is shown that the anisotropic parts of the different estimates of the effective stiffnesses are irreducible. A set of four discrete crystal orientations is presented, which ensures the isotropy of the effective elastic properties, i.e., a vanishing of the harmonic parts of different averages.

Keywords: B. Anisotropic material; B. Elastic material; B. Inhomogeneous material; A. Microstructures; B. Polycrystalline material

1. Introduction

Many materials are polycrystals consisting of a large number of crystalline grains. The effective properties of such aggregates are dominated by the statistical characteristics of the microstructure, e.g., the orientation distributions of the crystal lattice, the grain boundary surfaces, and grain edges. In most cases, the distribution of crystal orientations is of prime importance. Deviations from a uniform crystal orientation distribution cause the effective mechanical or physical properties to be anisotropic (Kocks et al., 1998). Usually, for a given crystal orientation distribution, one needs to determine the corresponding macroscopic properties. In the present paper, our concern is to find orientations that guarantee isotropic effective properties, where only the elastic

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properties are considered. The main purpose is to formulate an isotropy condition for aggregates of cubic crystals and to construct exact solutions of that condition with the minimal number of crystal orientations.

The outline of the paper is as follows. In Section 2, the harmonic decomposition of the elasticity tensors is specified for the case of cubic single crystals. In Section 3, different averages based on the orientation distribution function are used in order to give simple estimates of the effective elastic properties of textured polycrystals. These estimates correspond to the arithmetic, geometric, and harmonic averages of the stiffness tensors. This approach, although less accurate than more sophisticated averaging schemes like the self-consistent estimates or finite element calculations, allows the derivation of simple expressions describing the macroscopic anisotropy in terms of the microstructure and gives a first insight into the dominating mechanisms. In the case of aggregates of cubic crystals, the harmonic decomposition of all these averages consists of isotropic parts corresponding to a dilatational and a distortional deformation mode, and a complete symmetric and traceless fourth-order tensor with nine independent components. The reduction in the number of independent elastic constants on the macroscale from 21 (general triclinic) to 11 is caused by the cubic crystal symmetry on the microscale. In Section 4, we discuss the case when the orientation distribution function is such that all of the aforementioned effective stiffness tensors are isotropic. An exact solution based only on four single crystals with equal volumes is presented.

Throughout the text the summation convention is used. Linear mappings between second-order tensors are written as $\boldsymbol{A}=\mathbb{C}[\boldsymbol{B}]$. The scalar product, the dyadic product, and the Frobenius norm are denoted by $\boldsymbol{A}\cdot\boldsymbol{B}$, $\boldsymbol{A}\otimes\boldsymbol{B}$, and $||\boldsymbol{A}||=(\boldsymbol{A}\cdot\boldsymbol{A})^{1/2}$, respectively. Orth represents the set of proper orthogonal second-order tensors (special orthogonal group). Irreducible, i.e., complete symmetric and traceless tensors are provided with a prime, e.g. $\mathbb{C}'$. The basic isotropic second-, fourth-, and sixth-order tensors (Zheng and Betten, 1995) are denoted by $\boldsymbol{I}$, $\mathbb{I}$, and $\mathbb{J}$, respectively

$$\boldsymbol{I}=\boldsymbol{e}_i\otimes\boldsymbol{e}_i,\qquad \mathbb{I}=\tfrac{1}{2}\boldsymbol{e}_i\otimes\boldsymbol{e}_j\otimes(\boldsymbol{e}_i\otimes\boldsymbol{e}_j+\boldsymbol{e}_j\otimes\boldsymbol{e}_i), \tag{1}$$

$$\mathbb{J}=\tfrac{1}{8}(\boldsymbol{e}_i\otimes\boldsymbol{e}_j+\boldsymbol{e}_j\otimes\boldsymbol{e}_i)\otimes(\boldsymbol{e}_j\otimes\boldsymbol{e}_k+\boldsymbol{e}_k\otimes\boldsymbol{e}_j)\otimes(\boldsymbol{e}_k\otimes\boldsymbol{e}_i+\boldsymbol{e}_i\otimes\boldsymbol{e}_k), \tag{2}$$

$\{\boldsymbol{e}_i\}$ being an orthonormal basis.

The Rayleigh product $\boldsymbol{A}\bigstar\mathbb{C}$ of a second-order tensor $\boldsymbol{A}=A_{ij}\boldsymbol{e}_i\otimes\boldsymbol{e}_j$ and a fourth-order tensor $\mathbb{C}=C_{ijkl}\boldsymbol{e}_i\otimes\boldsymbol{e}_j\otimes\boldsymbol{e}_k\otimes\boldsymbol{e}_l$ is defined by

$$\boldsymbol{A}\bigstar\mathbb{C}=C_{ijkl}\boldsymbol{A}\boldsymbol{e}_i\otimes\boldsymbol{A}\boldsymbol{e}_j\otimes\boldsymbol{A}\boldsymbol{e}_k\otimes\boldsymbol{A}\boldsymbol{e}_l. \tag{3}$$

2. Elastic properties of single crystals

In classical elasticity, the stress tensor $\boldsymbol{T}$ is given as a linear map of the strain tensor $\boldsymbol{E}$ (Hooke's law), and vice versa

$$\boldsymbol{T}=\mathbb{C}[\boldsymbol{E}],\qquad \boldsymbol{E}=\mathbb{S}[\boldsymbol{T}]. \tag{4}$$

For hyperelastic materials, the elasticity tensors possess the major symmetry. The symmetry in the first and last pair of indices is assumed for convenience as usual. The

fourth-order stiffness tensor $\mathbb{C}$ and the corresponding compliance tensor $\mathbb{S}$ are specified by the symmetry group $\mathscr{S}$ of the material being a subgroup of the special orthogonal group, e.g., in terms of stiffnesses

$$\mathbb{C} = \boldsymbol{H} \star \mathbb{C}, \quad \forall \boldsymbol{H} \in \mathscr{S} \subseteq \mathrm{Orth}. \tag{5}$$

As mentioned by Forte and Vianello (1996), to each symmetry transformation $\boldsymbol{H} \in \mathrm{Orth}$ corresponds to $-\boldsymbol{H}$. Therefore, it is sufficient to consider a priori only symmetry transformations with a positive determinant. All kinds of physically possible two- and three-dimensional symmetry groups have been classified by Zheng and Boehler (1994). Forte and Vianello (1996) classified all the different forms of the linear operators $\mathbb{C}$ due to three-dimensional symmetry groups and showed that in the context of fourth-order linear operators only eight different symmetry classes can be distinguished.

Due to the major symmetry of the elasticity tensors, the following projector representations exist (Halmos, 1958; Rychlewski, 1995)

$$\mathbb{C} = \sum_{\alpha=1}^{\beta} \lambda_\alpha \mathbb{P}_\alpha, \qquad \mathbb{S} = \sum_{\alpha=1}^{\beta} \frac{1}{\lambda_\alpha} \mathbb{P}_\alpha. \tag{6}$$

Here, β $(2 \leqslant \beta \leqslant 6)$ is the number of distinct eigenvalues λ_α of $\mathbb{C}$. The projectors $\mathbb{P}_\alpha$ map each symmetric second-order tensor into the αth eigenspace of $\mathbb{C}$. They are idempotent $\mathbb{P}_\alpha \mathbb{P}_\alpha = \mathbb{P}_\alpha$, biorthogonal $\mathbb{P}_\alpha \mathbb{P}_\gamma = \mathbb{O}$ $(\alpha \neq \gamma)$, and complete $\sum_{\alpha=1}^{\beta} \mathbb{P}_\alpha = \mathbb{I}$. In the case of isotropy, i.e. $\mathscr{S} = \mathrm{Orth}$, only two different projectors exist

$$\mathbb{P}_1^I = \tfrac{1}{3} \boldsymbol{I} \otimes \boldsymbol{I}, \qquad \mathbb{P}_2^I = \mathbb{I} - \mathbb{P}_1^I. \tag{7}$$

It is possible to decompose all elasticity tensors of arbitrary symmetry into a direct sum of orthogonal subspaces

$$\mathbb{C} = h_1 \mathbb{P}_1^I + h_2 \mathbb{P}_2^I + \boldsymbol{H}_1' \otimes \boldsymbol{I} + \boldsymbol{I} \otimes \boldsymbol{H}_1' + 4\mathbb{J}[\boldsymbol{H}_2'] + \mathbb{H}', \tag{8}$$

where $\boldsymbol{H}_1'$, $\boldsymbol{H}_2'$, and $\mathbb{H}'$ are irreducible, i.e., completely symmetric and traceless, tensors. This representation is called the harmonic decomposition of fourth-order tensors (Schouten, 1924; Spencer, 1970; Cowin, 1989; Boehler et al., 1994; for an overview see Forte and Vianello, 1996). $h_{1,2}$ are called the first and second isotropic parts, $\boldsymbol{H}_{1,2}'$ the first and second deviatoric parts, and $\mathbb{H}'$ the harmonic part. Irreducible second-order tensors have five and irreducible fourth-order tensors have nine independent components.

In the following, we consider the case of a cubic crystal symmetry. In this case, $\mathscr{S}$ consists of 24 elements. They are given here with respect to the orthonormal crystal lattice vector $\{\boldsymbol{g}_i\}$: (1) the identity; (2) rotations of order 2 about the axes $(\boldsymbol{g}_i \pm \boldsymbol{g}_j)/\sqrt{2}$, $(i < j)$; (3) rotations of order 3 about the axes $(\boldsymbol{g}_1 \pm \boldsymbol{g}_2 \pm \boldsymbol{g}_3)/\sqrt{3}$; and (4) rotations of order 4 about the axes $\boldsymbol{g}_i$ $(i = 1,2,3)$ and their powers of order 2 and 3. The angle of the rotation is determined by $\vartheta = 2\pi/k$, k being the order of the rotation.

The cubic elasticity tensors have three distinct eigenvalues $(\beta = 3)$ which can be given by the components of $\mathbb{C}$ with respect to the lattice vectors $\{\boldsymbol{g}_i\}$ $(i = 1,2,3)$:

$\lambda_1 = C_{1111} + 2C_{1122}$, $\lambda_2 = C_{1111} - C_{1122}$, and $\lambda_3 = 2C_{1212}$. The cubic projectors (Rychlewski and Zhang, 1989; Bertram and Olschewski, 1991) are

$$\mathbb{P}_1^C = \mathbb{P}_1^I, \qquad \mathbb{P}_2^C = \mathbb{D} - \mathbb{P}_1^C, \qquad \mathbb{P}_3^C = \mathbb{I} - \mathbb{P}_2^C - \mathbb{P}_1^C. \tag{9}$$

The anisotropic part $\mathbb{D}$ is specified by a dyadic product of lattice vectors

$$\mathbb{D} = \sum_{i=1}^{3} \boldsymbol{g}_i \otimes \boldsymbol{g}_i \otimes \boldsymbol{g}_i \otimes \boldsymbol{g}_i. \tag{10}$$

The symmetry group of $\mathbb{C}$ is the intersection of the symmetry groups of its harmonic and deviatoric parts (Forte and Vianello, 1996). As a result, cubic symmetry forces $\boldsymbol{H}'_{1,2} = \gamma_{1,2}\boldsymbol{I}$, and from $\mathrm{tr}(\boldsymbol{H}'_{1,2}) = 0$ one concludes that $\gamma_{1,2} = 0$. Therefore, the tensors $\boldsymbol{H}'_{1,2}$ vanish and the harmonic decomposition of the single crystal stiffness reduces to

$$\mathbb{C} = h_1\mathbb{P}_1^I + h_2\mathbb{P}_2^I + \mathbb{H}'. \tag{11}$$

The first and second isotropic parts $h_{1,2}$ are determined by a projection of $\mathbb{C}$ onto the space of isotropic fourth-order tensors, i.e.

$$h_\gamma = \mathbb{C} \cdot \frac{\mathbb{P}_\gamma^I}{||\mathbb{P}_\gamma^I||^2}, \quad \gamma = 1, 2. \tag{12}$$

From Eqs. (7), (9), (11), and (12) the harmonic part $\mathbb{H}'$ can be determined. As a result, the following relations hold

$$h_1 = \lambda_1, \quad h_2 = \frac{2}{5}\lambda_2 + \frac{3}{5}\lambda_3, \quad \boldsymbol{H}'_{1,2} = \boldsymbol{0}, \quad \mathbb{H}' = \frac{1}{5}(\lambda_3 - \lambda_2)(\boldsymbol{I} \otimes \boldsymbol{I} + 2\mathbb{I} - 5\mathbb{D}). \tag{13}$$

3. Effective elastic properties

Based on the orientation distribution function f defined on Orth, different orientation averages of elasticity tensors can be introduced. The most common mean values are the arithmetic and the harmonic means of the local stiffness tensors, which were first suggested by Voigt and Reuss, respectively

$$\mathbb{C}^V = \int_g f(g)\mathbb{C}(g)\,\mathrm{d}g, \qquad \mathbb{S}^R = \int_g f(g)\mathbb{S}(g)\,\mathrm{d}g \neq \mathbb{C}^{V-1}, \tag{14}$$

$\mathrm{d}g$ being the volume element in Orth (Voigt, 1928; Reuss, 1929; Bunge, 1968; Morris, 1969). The arithmetic and the harmonic means correspond to the assumption of homogeneous strain and stress fields, respectively. These approaches give upper and lower bounds for the strain energy density (Hill, 1952; Nemat-Nasser and Hori, 1993).

An approach that focuses on homogenization resulting in unique effective properties, such that the inverse of the effective compliance is equal to the effective stiffness, was given by Aleksandrov and Aisenberg (1966) and further developed by Matthies and Humbert (1995). Here, the geometric mean of the local elastic moduli is used

$$\mathbb{C}^A = \exp\left(\int_g f(g)\ln(\mathbb{C}(g))\,\mathrm{d}g\right), \qquad \mathbb{S}^A = \exp\left(\int_g f(g)\ln(\mathbb{S}(g))\,\mathrm{d}g\right) \equiv \mathbb{C}^{A-1}. \tag{15}$$

The natural logarithm is applied to the eigenvalues of $\mathbb{C}$ and $\mathbb{S}$, as usual. Predictions based on this approach are similar to self-consistent estimates and close to experimental data (Matthies and Humbert, 1995).

For a uniform distribution of crystal orientations, $f(g)=1$ holds for all $g\in\mathrm{Orth}$, and the integrals

$$\mathbb{C}^{VI}=\int_g \mathbb{C}(g)\,\mathrm{d}g,\quad \mathbb{C}^{AI}=\exp\left(\int_g \ln(\mathbb{C}(g))\,\mathrm{d}g\right),\quad \mathbb{S}^{RI}=\int_g \mathbb{S}(g)\,\mathrm{d}g \tag{16}$$

can be expressed solely in terms of the single crystal constants.

Based on the aforementioned formulae, it is possible to decompose the generally anisotropic averages into isotropic and anisotropic parts

$$\begin{aligned}&\mathbb{C}^V=\mathbb{C}^{VI}+\zeta^V\mathbb{A}^V,\\ &\ln(\mathbb{C}^A)=\ln(\mathbb{C}^{AI})+\zeta^A\mathbb{A}^A,\\ &\mathbb{S}^R=\mathbb{S}^{RI}+\zeta^R\mathbb{A}^R.\end{aligned} \tag{17}$$

By definition, the norms $||\mathbb{A}^{V,A,R}||$ are zero for a uniform orientation distribution. The scalars $\zeta^{V,A,R}$ may be defined such that the norms $||\mathbb{A}^{V,A,R}||$ are equal to one for a single crystal orientation.

For aggregates of cubic crystals, the arithmetic mean $(14)_1$ reads (see Eqs. (11) and (13))

$$\begin{aligned}\mathbb{C}^V&=\int_g f(g)\mathbb{C}(g)\,\mathrm{d}g\\ &=h_1\mathbb{P}_1^I+h_2\mathbb{P}_2^I+\int_g f(g)\mathbb{H}'(g)\,\mathrm{d}g\\ &=\lambda_1\mathbb{P}_1^I+\left(\frac{2}{5}\lambda_2+\frac{3}{5}\lambda_3\right)\mathbb{P}_2^I+\frac{1}{5}(\lambda_3-\lambda_2)\left(\boldsymbol{I}\otimes\boldsymbol{I}+2\mathbb{I}-5\int_g f(g)\mathbb{D}(g)\,\mathrm{d}g\right).\end{aligned} \tag{18}$$

In a similar way, the geometric and the harmonic means are obtained

$$\begin{aligned}\ln(\mathbb{C}^A)&=\ln(\lambda_1)\mathbb{P}_1^I+\ln(\lambda_2^{2/5}\lambda_3^{3/5})\mathbb{P}_2^I+\tfrac{1}{5}(\ln(\lambda_3)-\ln(\lambda_2))\\ &\quad\times\left(\boldsymbol{I}\otimes\boldsymbol{I}+2\mathbb{I}-5\int_g f(g)\mathbb{D}(g)\,\mathrm{d}g\right),\\ \mathbb{S}^R&=\frac{1}{\lambda_1}\mathbb{P}_1^I+\left(\frac{2}{5}\frac{1}{\lambda_2}+\frac{3}{5}\frac{1}{\lambda_3}\right)\mathbb{P}_2^I+\frac{1}{5}\left(\frac{1}{\lambda_3}-\frac{1}{\lambda_2}\right)\\ &\quad\times\left(\boldsymbol{I}\otimes\boldsymbol{I}+2\mathbb{I}-5\int_g f(g)\mathbb{D}(g)\,\mathrm{d}g\right).\end{aligned} \tag{19}$$

It can be easily seen that for a single crystal orientation

$$\left|\left|\boldsymbol{I}\otimes\boldsymbol{I}+2\mathbb{I}-5\int_g f(g)\mathbb{D}(g)\,\mathrm{d}g\right|\right|=\sqrt{30} \tag{20}$$

holds. Therefore, for aggregates of cubic crystals, the scalar factors in Eqs. (17) are given by

$$\zeta^V = \sqrt{\tfrac{6}{5}}(\lambda_3 - \lambda_2), \quad \zeta^A = \sqrt{\tfrac{6}{5}}(\ln(\lambda_3) - \ln(\lambda_2)), \quad \zeta^R = \sqrt{\tfrac{6}{5}}\left(\frac{1}{\lambda_3} - \frac{1}{\lambda_2}\right). \tag{21}$$

Moreover, from Eqs. (18), (19), and (21) it follows that

$$\mathbb{A}^V = \mathbb{A}^A = \mathbb{A}^R =: \mathbb{A}', \tag{22}$$

where

$$\mathbb{A}' = \frac{\sqrt{30}}{30}\left(\boldsymbol{I}\otimes\boldsymbol{I} + 2\mathbb{I} - 5\int_g f(g)\mathbb{D}(g)\,\mathrm{d}g\right) \tag{23}$$

(Bertram and Böhlke, 1999). Inspection shows that the tensor $\mathbb{A}'$ is irreducible, i.e., completely symmetric and traceless

$$A'_{ijkl} = A'_{jikl} = A'_{klij} = A'_{kjil} = \cdots, \qquad A'_{iike} = 0. \tag{24}$$

A harmonic decomposition of the different averages (14) and (15) is obtained in a similar way as in the case of single crystals. Comparison of Eqs. (8), (11), and (14) gives the arithmetic mean

$$\mathbb{C}^V = h_1^V\mathbb{P}_1^I + h_2^V\mathbb{P}_2^I + \boldsymbol{H}_1'^V\otimes\boldsymbol{I} + \boldsymbol{I}\otimes\boldsymbol{H}_1'^V + 4\mathbb{J}[\boldsymbol{H}_2'^V] + \mathbb{H}'^V, \tag{25}$$

where

$$h_1^V = h_1, \quad h_2^V = h_2, \quad \boldsymbol{H}_{1,2}'^V = \boldsymbol{0}, \quad \mathbb{H}' = \zeta^V\mathbb{A}'. \tag{26}$$

In order to determine the elastic anisotropy experimentally, in most cases Young's modulus E is measured in tensile tests. E is defined as the ratio of stress and strain in the tensile direction $\boldsymbol{d}$ which in the case of the harmonic mean is equivalent to

$$\begin{aligned}\frac{1}{E^R(\boldsymbol{d})} &= \boldsymbol{d}\otimes\boldsymbol{d}\cdot\mathbb{S}^R[\boldsymbol{d}\otimes\boldsymbol{d}]\\ &= \tfrac{1}{3}h_1^R + \tfrac{2}{3}h_2^R + \zeta^R\boldsymbol{d}\otimes\boldsymbol{d}\cdot\mathbb{A}'[\boldsymbol{d}\otimes\boldsymbol{d}],\end{aligned} \tag{27}$$

$h_{1,2}^R$ being the isotropic parts of the harmonic decomposition of $\mathbb{S}^R$. Experiments confirm that the tensor $\mathbb{A}'$ actually represents the elastic anisotropy. Texture data of rolled copper have been used to determine the Voigt and Reuss average as well as the Hill approximation of Young's modulus (Alers and Liu, 1966; Kallend and Davies, 1971). A comparison of these predictions with the measured modulus shows that the absolute value of Young's modulus strongly depends on the type of the average, but the variation of the modulus with respect to the sample orientation, i.e. $E(\boldsymbol{d})$, is not very sensitive to the type of average and corresponds to the experimental findings.

It is well known that for each of the 32 crystal symmetry groups and the five transversely isotropic groups a single tensor can be constructed that characterizes this group (Zheng and Spencer, 1993). Here, the single tensor $\mathbb{A}'$ covers all possible cases of symmetries that can be induced by a texture in an aggregate of cubic crystals, e.g., a triclinic behavior, orthotropy, or isotropy. This description of anisotropy differs from the method based on second-order structure tensors (Boehler, 1987), where the number of structure tensors depends on the specific symmetry to be modeled. In Bertram

and Böhlke (1999) the texture induced elastic anisotropy is studied numerically for polycrystalline copper. In Böhlke and Bertram (2001) an evolution equation for $\mathbb{A}'$ is formulated based on the theory of isotropic tensor functions in order to describe the texture induced elastic anisotropy that accompanies metal forming operations.

The decomposition (17) with the special properties (22) and (24) may be considered from the point of a Fourier series expansion of the distribution function of crystal orientations $f(g)$. If $f(g)$ is continuous and square integrable over Orth then it can be represented by a Fourier series (Adams et al., 1992; Bunge, 1993). Moreover, the generalized spherical harmonics constitute a complete orthogonal basis for the continuous and square integrable functions over Orth. The tensor spherical harmonics of the expansion are irreducible, i.e. completely symmetric and traceless. The Fourier series expansion of $f(g)$ in the case of aggregates of cubic crystals has the property that only even-rank spherical harmonics occur and that the first tensor spherical harmonic is of rank four (Adams et al., 1992; Bunge, 1993). Since the strain energy density of the polycrystal is expected to be governed by the tensor coefficients of that expansion, the decomposition of the elasticity tensors in an isotropic and a fourth-order irreducible anisotropic part corresponds to the Fourier series expansion.

4. Discrete isotropic orientation distributions

In the previous section, it was shown that in the case of aggregates of cubic crystals the effective elastic behavior was completely determined by 11 constants. Two parameters describe the isotropic behavior and the other nine reflect the influence of the crystallographic texture. The reduction in the number of independent elastic constants on the macroscale from 21 (general triclinic) to 11 (reduced triclinic) is caused by the cubic crystal symmetry on the microscale. In this section, we present a set of discrete orientations that satisfy the isotropy condition (Böhlke and Bertram, 1999)

$$\mathbb{A}' = \mathbb{O}, \tag{28}$$

which gives isotropic arithmetic, geometric, and harmonic means.

The averages (14) and (15) can be regarded as special cases of power means (e.g., Marcus and Minc, 1992) which are applied to positive definite fourth-order tensors. Inspection shows that the isotropy condition (28) holds irrespective of the order of the power mean. Hence, the sets of crystal orientations satisfying Eq. (28) guarantee isotropic effective elastic properties for a broad class of micromechanical estimates.

Due to the above mentioned irreducibility of $\mathbb{A}'$, Eq. (28) contains nine independent equations. The irreducibility of $\mathbb{A}'$ is equivalent to the following constraints upon its components:

$$\begin{aligned}
&A'_{45} = \sqrt{2}A'_{36}, && A'_{11} + A'_{12} + A'_{13} = 0,\\
&A'_{46} = \sqrt{2}A'_{25}, && A'_{12} + A'_{22} + A'_{23} = 0,\\
&A'_{56} = \sqrt{2}A'_{14}, && A'_{13} + A'_{23} + A'_{33} = 0,\\
&A'_{44} = 2A'_{23}, && A'_{14} + A'_{24} + A'_{34} = 0,
\end{aligned}$$

$$\begin{aligned} A'_{55} &= 2A'_{13}, \qquad A'_{15} + A'_{25} + A'_{35} = 0, \\ A'_{66} &= 2A'_{12}, \qquad A'_{16} + A'_{26} + A'_{36} = 0. \end{aligned} \tag{29}$$

The components $A'_{\alpha\beta} = \boldsymbol{B}_\alpha \cdot \mathbb{A}'[\boldsymbol{B}_\beta]$ refer to the orthonormal basis $\boldsymbol{B}_\alpha$ of a six-dimensional space (Federov, 1968; Cowin, 1990)

$$\begin{aligned} \boldsymbol{B}_1 &= \boldsymbol{e}_1 \otimes \boldsymbol{e}_1, \qquad \boldsymbol{B}_4 = \frac{\sqrt{2}}{2}(\boldsymbol{e}_2 \otimes \boldsymbol{e}_3 + \boldsymbol{e}_3 \otimes \boldsymbol{e}_2), \\ \boldsymbol{B}_2 &= \boldsymbol{e}_2 \otimes \boldsymbol{e}_2, \qquad \boldsymbol{B}_5 = \frac{\sqrt{2}}{2}(\boldsymbol{e}_1 \otimes \boldsymbol{e}_3 + \boldsymbol{e}_3 \otimes \boldsymbol{e}_1), \\ \boldsymbol{B}_3 &= \boldsymbol{e}_3 \otimes \boldsymbol{e}_3, \qquad \boldsymbol{B}_6 = \frac{\sqrt{2}}{2}(\boldsymbol{e}_1 \otimes \boldsymbol{e}_2 + \boldsymbol{e}_2 \otimes \boldsymbol{e}_1). \end{aligned} \tag{30}$$

A formulation of the tensor $\mathbb{D}$ with respect to the basis $\{\boldsymbol{e}_i\}$ is obtained by introducing the orthogonal tensor $\boldsymbol{Q} = \boldsymbol{g}_i \otimes \boldsymbol{e}_i = Q_{ij}\boldsymbol{e}_i \otimes \boldsymbol{e}_j$ that maps the basis $\{\boldsymbol{e}_i\}$ onto the crystallographic basis $\{\boldsymbol{g}_i\}$

$$D_{ijmn} = \sum_{k=1}^{3} Q_{ik}Q_{jk}Q_{mk}Q_{nk}. \tag{31}$$

If only discrete orientations are considered, the average over the orientation space can be formulated as a weighted sum

$$\int_g f(g)\mathbb{D}(g)\,\mathrm{d}g = \sum_{\alpha=1}^{N} \upsilon^\alpha \mathbb{D}(g^\alpha), \tag{32}$$

υ^α being the volume fraction corresponding to the orientation g^α. N denotes the total number of orientations. Then the isotropy condition (28) reads

$$\delta_{ij}\delta_{mn} + \delta_{im}\delta_{jn} + \delta_{in}\delta_{jm} - 5\sum_{\alpha=1}^{N} \upsilon^\alpha \sum_{k=1}^{3} Q^\alpha_{ik}Q^\alpha_{jk}Q^\alpha_{mk}Q^\alpha_{nk} = 0. \tag{33}$$

Each of the orientations $\boldsymbol{Q}^\alpha$ has three independent components as a result of the orthogonality condition.

In Bertram et al. (2000) Eq. (28) is discussed in a group theoretical context. In that work, it is shown that exact solutions of Eq. (28) can be generally found for N grains with equal size ($\upsilon^\alpha = 1/N$) for all even N larger than 3. In this paper, such a minimal solution for $N = 4$ is derived by a different method. Eq. (28) can be solved numerically with the first orientation being equal to the identity tensor, so that nine degrees of freedom remain corresponding to the nine independent components of $\mathbb{A}'$. The numerical solutions are of the following kind:

$$Q^{\mathrm{I}}_{ij} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad Q^{\mathrm{II}}_{ij} = \begin{bmatrix} +p_1 & -p_5 & -p_4 \\ -p_2 & +p_3 & -p_5 \\ +p_6 & +p_2 & -p_1 \end{bmatrix},$$

$$Q_{ij}^{\mathrm{III}} = \begin{bmatrix} -p_5 & +p_2 & +p_3 \\ -p_1 & -p_6 & +p_2 \\ +p_4 & +p_1 & +p_5 \end{bmatrix}, \quad Q_{ij}^{\mathrm{IV}} = \begin{bmatrix} -p_2 & +p_1 & +p_6 \\ -p_5 & -p_4 & -p_1 \\ +p_3 & -p_5 & +p_2 \end{bmatrix}, \tag{34}$$

with the property $p_1 + p_2 = p_5$ of the components occurring twice. These constraints, indicated by the numerical solutions, allow the complete determination of a solution with $N = 4$.

The quaternion representation of orthogonal tensors is convenient for the subsequent argumentation and implies for the orientation $\boldsymbol{Q}^{\mathrm{II}}$

$$Q_{ij}^{\mathrm{II}} = \begin{bmatrix} y_1^2 + y_2^2 - y_3^2 - y_4^2 & -2y_1y_4 + 2y_2y_3 & 2y_1y_3 + 2y_2y_4 \\ 2y_1y_4 + 2y_2y_3 & y_1^2 - y_2^2 + y_3^2 - y_4^2 & -2y_1y_2 + 2y_3y_4 \\ -2y_1y_3 + 2y_2y_4 & 2y_1y_2 + 2y_3y_4 & y_1^2 - y_2^2 - y_3^2 + y_4^2 \end{bmatrix} \tag{35}$$

with

$$y_1^2 + y_2^2 + y_3^2 + y_4^2 = 1. \tag{36}$$

The constraints given by Eq. $(34)_2$, i.e. $Q_{21}^{\mathrm{II}} = -Q_{32}^{\mathrm{II}}$, $Q_{11}^{\mathrm{II}} = -Q_{33}^{\mathrm{II}}$, and $Q_{12}^{\mathrm{II}} = Q_{23}^{\mathrm{II}}$, are fulfilled identically by setting $y_1 = -y_3$. With the substitutions $y_3 = \sqrt{r}\sin(\phi)/\sqrt{2}$ and $y_4 = \sqrt{r}\cos(\phi)$, Eq. (36) gives $y_2 = \sqrt{1-r}$. One of the two remaining unknowns r and ϕ can be eliminated with the aforementioned constraint $p_1 + p_2 = p_5$, i.e. $-Q_{12}^{\mathrm{II}} + Q_{21}^{\mathrm{II}} - Q_{11}^{\mathrm{II}} = 0$. One obtains

$$r = \frac{1}{1 + \cos^2(\phi) - 2\sqrt{2}\sin(\phi)\cos(\phi)} \tag{37}$$

or, with $z = \tan(\phi)$, equivalently

$$r = \frac{z^2 + 1}{z^2 - 2z\sqrt{2} + 2}. \tag{38}$$

Now y_i read

$$y_1 = -y_3 = \frac{\sqrt{2}}{2}\frac{z}{z - \sqrt{2}}, \quad y_2 = \frac{1}{2}\frac{\sqrt{2\sqrt{2}(\sqrt{2} - 4z)}}{\sqrt{2} - z}, \quad y_4 = \frac{1}{\sqrt{2} - z}. \tag{39}$$

By substituting Eq. (39) into Eqs. (35) and (34) the Frobenius norm of $\mathbb{A}'$ reduces to

$$||\mathbb{A}'|| = \frac{z^3 + 7z^2\sqrt{2} + 6z - 2\sqrt{2}}{(z - \sqrt{2})^3}. \tag{40}$$

The discriminant of the cubic polynomial in the numerator has the value $D = -2600/27$. Since the discriminant is negative, three real solutions exist. They have the following values

$$z_1 = \frac{8}{3}\sqrt{5}\cos\left(\frac{1}{3}\pi - \frac{1}{3}\arccos\left(\frac{47}{160}\sqrt{2}\sqrt{5}\right)\right) - \frac{7}{3}\sqrt{2},$$

$$z_2 = -\frac{8}{3}\sqrt{5}\cos\left(\frac{1}{3}\arccos\left(\frac{47}{160}\sqrt{2}\sqrt{5}\right)\right) - \frac{7}{3}\sqrt{2},$$

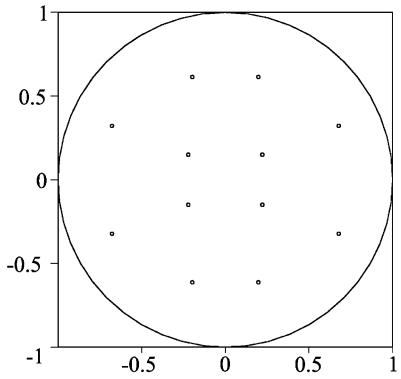

Fig. 1. $\{1\,0\,0\}$ pole figure.

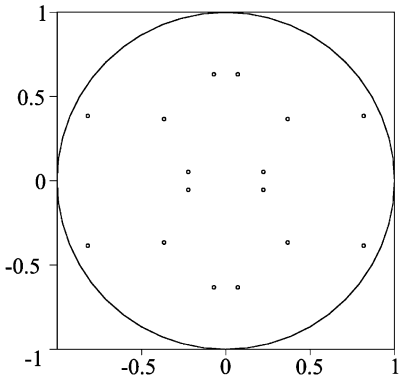

Fig. 2. $\{1\,1\,1\}$ pole figure.

$$z_3 = \frac{8}{3}\sqrt{5}\sin\left(\frac{1}{6}\pi - \frac{1}{3}\arccos\left(\frac{47}{160}\sqrt{2}\sqrt{5}\right)\right) - \frac{7}{3}\sqrt{2}. \tag{41}$$

The symmetry group $\mathscr{S}$ induces equivalent crystal orientations by

$$\boldsymbol{g}_i \equiv \boldsymbol{H}\boldsymbol{g}_i, \quad \forall \boldsymbol{H} \in \mathscr{S} \subseteq \mathrm{Orth} \quad \Leftrightarrow \quad \boldsymbol{Q} \equiv \boldsymbol{H}\boldsymbol{Q}, \quad \forall \boldsymbol{H} \in \mathscr{S} \subseteq \mathrm{Orth}. \tag{42}$$

The three solutions $z_{1,2,3}$ are equivalent in the sense that the corresponding sets of orthogonal matrices $\boldsymbol{Q}^{\alpha}_{1,2,3}$ $(\alpha = \mathrm{I}, \mathrm{II}, \mathrm{III}, \mathrm{IV})$ can be transformed by elements of $\mathscr{S}$ such that $\boldsymbol{Q}^{\alpha}_1 = \boldsymbol{Q}^{\alpha}_2 = \boldsymbol{Q}^{\alpha}_3$ $(\alpha = \mathrm{I}, \mathrm{II}, \mathrm{III}, \mathrm{IV})$ hold.

In Figs. 1 and 2, the $\{1\,0\,0\}$ and the $\{1\,1\,1\}$ pole figures of this exact solution are shown. In Fig. 3, a three-dimensional plot of cubes representing the four crystal orientations is given.

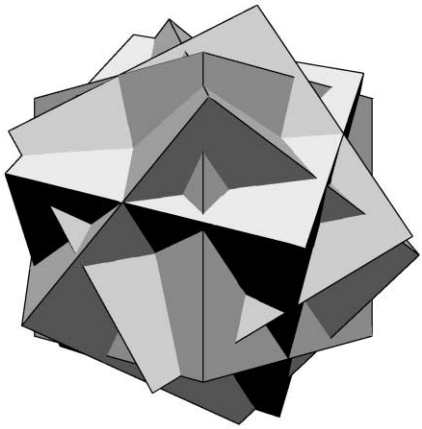

Fig. 3. Three-dimensional plot of cubes representing the four crystal orientations.

5. Conclusions

It is shown that certain parts of the harmonic decomposition of the effective stiffnesses vanish as a result of the cubic symmetry of the constituents forming the aggregate. An isotropy condition is formulated for aggregates of cubic crystals. An exact solution with the minimal number of crystal orientations is presented. Solutions of that kind can be used as input data for micro-macro simulations based on Taylor-type models or finite element approaches.

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