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DESIGNING TEXTURED POLYCRYSTALS WITH SPECIFIC ISOTROPIC MATERIAL TENSORS: THE ODF METHOD

Abstract. Herein we study the following problem: Suppose we are given a supply of grains, which are of the same material and have equal volume. Given a finite set of material tensors $\mathbb{H}^{(i)}$, can we find an arrangement of grains in an aggregate so that all the tensors $\mathbb{H}^{(i)}$ pertaining to this aggregate are isotropic? In this paper we examine the preceding problem within the special context of physical theories where material anisotropy of polycrystalline aggregates is determined by crystallographic texture, and we restrict our attention to tensors whose anisotropic part is linear in the texture coefficients. A method is developed by which the preceding problem is answered positively for tensors of various orders and grains of various crystal symmetries. Our method uses the machinery developed in quantitative texture analysis. It is based on the symmetry properties of the orientation distribution function (ODF) and appeals to some recent findings on how crystallographic texture affects material tensors of weakly textured polycrystals. As illustration, explicit solutions are worked out for the fourth-order elasticity tensor and for the sixth-order acoustoelastic tensor.

1. Introduction

Consider an aggregate $\mathcal{A}$ of N linearly elastic cubic crystallites $\mathcal{B}_\alpha$, which are of the same material and have equal volume. Let a reference crystallite $\mathcal{B}_o$ be chosen, and let $\mathbb{C}^o$ be its elasticity tensor. For a rotation R and fourth-order tensor $\mathbb{H}$, let $R^{\otimes 4}$ be the linear transformation on the space of fourth-order tensors such that $\widetilde{\mathbb{H}} \equiv R^{\otimes 4}\mathbb{H}$ has its Cartesian components given by

$$\widetilde{H}_{ijkl} = R_{ip} R_{jq} R_{kr} R_{ls} H_{pqrs},$$

where R_{ij} and H_{pqrs} denote the components of R and of $\mathbb{H}$, respectively, and repeated suffixes mean summation from 1 to 3. Under the Voigt model, the effective elasticity tensor of the aggregate $\mathcal{A}$ is given by

$$\overline{\mathbb{C}} = \frac{1}{N} \sum_{\alpha=1}^{N} R_\alpha^{\otimes 4} \mathbb{C}^o, \tag{1}$$

where the rotation R_α defines the orientation of $\mathcal{B}_\alpha$ with respect to $\mathcal{B}_o$. Recently Bertram et al. [1, 2], in the course of their work on texture-induced elastic anisotropy that results from finite

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plastic deformations of polycrystals, raised and answered the following question: What is the smallest number N of cubic grains required and how should they be arranged (i.e., determine R_α for $\alpha = 1, 2, ..., N$) so that $\overline{\mathbb{C}}$ is isotropic? They proved that the smallest N is 4 and determined R_1, ..., R_4 for $\overline{\mathbb{C}}$ in Eq. (1) to be isotropic. In their papers Bertram et al. showed also that each arrangement R_α ($\alpha = 1, ..., N$) which delivers an isotropic $\overline{\mathbb{C}}$ under the Voigt model also renders the effective elasticity tensor isotropic under the Reuss model and under the "geometric mean" estimate [3, 4].

For broader applications, naturally one would ask analogous questions that pertain to aggregates of grains of other crystalline symmetries and to other material tensors. For example, the sixth-order acoustoelastic tensor [5, 6] figures prominently in problems that concern wave propagation in prestressed solids; in some formulations [7], yield functions and flow rules in plasticity involve not only fourth-order tensors but also sixth-order and even higher order tensors. For definiteness, let us paraphrase the problem that we shall investigate in this paper as follows: Suppose we are given an unlimited supply of grains $\mathcal{B}_\alpha$, which are of the same material, have equal volume, and have crystal symmetry characterized by the group $\mathcal{G}_{\rm cr}$. We consider aggregates $\mathcal{A}$ made up of a finite number N of grains $\mathcal{B}_\alpha$. Given a finite set of material tensors $\mathbb{H}^{(1)}, \ldots, \mathbb{H}^{(s)}$, find a number N and an arrangement of grains $\mathcal{B}_\alpha$ for which the N-grain aggregate $\mathcal{A}$ has all its tensors $\mathbb{H}^{(i)}$ ($i = 1, \ldots, s$) isotropic. To reduce the foregoing to a manageable mathematical problem, we shall restrict our discussion to a special class of physical theories where material anisotropy of polycrystalline aggregates is determined by crystallographic texture (i.e., the preferred orientations of the constituting grains), and we shall only consider what we call tensor functions of class (*) (see Definition 2 in Section 3 for a precise definition). Prime examples are tensors of polycrystals defined by orientational averaging (e.g., $\overline{\mathbb{C}}$ in Eq. (1)) and material tensors of "weakly textured" polycrystals [8, 9].

In their papers [1, 2], Bertram et al. restricted their attention to fourth-order tensors and to aggregates of grains with cubic symmetry. As far as we can discern, the methods that they developed are applicable only for those special circumstances. To tackle our more general problem, we shall appeal to the machinery developed in quantitative texture analysis [10, 11, 12], in particular the restrictions that crystal and texture symmetry impose on the orientation distribution function (ODF), and draw on some recent findings of Man [8, 13] with regard to how crystallographic texture affects material tensors of weakly textured polycrystals. Since the expansion coefficients c^l_{mn} of the ODF (see Eq. (9) in Section 2.2) play a crucial role in the present work, we call the approach developed in this paper for designing polycrystals with specific isotropic material tensors the *ODF method*.

As the reader will see in detail below, this method relies on finding suitable combinations of crystal and texture symmetries which produce solvable systems of equations where specific texture coefficients c^l_{mn} of an aggregate are set equal to zero. In this paper we take $\mathcal{G}_{\rm cr}$ to be a finite rotation group which satisfies the crystallographic restriction, i.e., $\mathcal{G}_{\rm cr} = C_1, C_2, C_3, C_4, C_6, D_2, D_3, D_4, D_6, T$, or O in the Schoenflies notation. Let $\mathcal{G}_{\rm tex}$ be a group of texture symmetry. Unlike $\mathcal{G}_{\rm cr}$, $\mathcal{G}_{\rm tex}$ need not observe the crystallographic restriction. The only requirement on $\mathcal{G}_{\rm tex}$ is that it be a subgroup of the rotation group. Since we shall use various $\mathcal{G}_{\rm tex}$'s for building aggregates that consist of a finite number of crystallites, in this paper we use only those $\mathcal{G}_{\rm tex}$ which are finite. In what follows, for a finite group G, we write $|G|$ for the order of G.

2. Preliminaries

In this section we recapitulate some facts about orientation measures and tensor representations of the rotation group, which we shall use below. Throughout this paper, when we talk about orientations of crystallites, it is understood that a reference crystallite has been chosen. The orientation of a crystallite is then specified by a rotation with respect to the reference.

2.1. Tensor representations of the rotation group

Let V be the translation space of the three-dimensional Euclidean space, and V^r the r-fold tensor product $V \otimes V \cdots \otimes V$. A rotation Q on V induces a linear transformation $Q^{\otimes r}$ on V^r defined by

$$(Q^{\otimes r}\mathbb{H})_{i_1\cdots i_r} = Q_{i_1 j_1} Q_{i_2 j_2} \cdots Q_{i_r j_r} H_{j_1\cdots j_r}, \tag{2}$$

where repeated suffixes mean summation from 1 to 3. The map $Q \mapsto Q^{\otimes r}$ defines [14] a linear representation of the rotation group SO(3) on V^r. A subspace $Z \subset V^r$ is said to be invariant under the action of the rotation group if it remains invariant under $Q^{\otimes r}$ for each rotation Q. Let $Q^{\otimes r}|Z$ be the restriction of $Q^{\otimes r}$ on Z. Then $Q \mapsto Q^{\otimes r}|Z$ defines a linear representation of the rotation group on Z. We refer to these representations of SO(3) on tensor spaces as tensor representations. By formally introducing the complexification V_c of V and Z_c of Z (see Miller [14], p. 105), we shall henceforth regard the tensor representations as complex representations. For simplicity, we shall suppress the subscript "c" and continue to write the complex representations as $Q \mapsto Q^{\otimes r}|Z$.

In what follows we shall be concerned only with tensor spaces Z which remain invariant under the action of the rotation group and, to specify the various types of tensors, we shall adopt a system of notation advocated by Jahn [15] and Sirotin [16]. In this notation, V^2 stands for the tensor product $V \otimes V$, $[V^2]$ the space of symmetric second-order tensors, $V[V^2]$ the tensor product of V and $[V^2]$, $[[V^2]^2]$ the symmetric square of $[V^2]$ (i.e., the symmetrized tensor product of $[V^2]$ and $[V^2]$), $[[V^2]^3]$ the symmetric cube of $[V^2]$, $[V^2][[V^2]^2]$ the tensor product of $[V^2]$ and $[[V^2]^2]$, ..., etc. For instance, the fourth-order elasticity tensor is of type $[[V^2]^2]$, and the sixth-order acoustoelastic tensor of type $[V^2][[V^2]^2]$.

Following usual practice [16], we shall use the notation for each type of tensor space (e.g., $[[V^2]^2]$) to denote also the corresponding tensor representation (e.g., $Q \mapsto Q^{\otimes 4}|[[V^2]^2]$). Whether we really mean the tensor space or the corresponding tensor representation should be clear from the context. The rotation group has a complete set of absolutely irreducible unitary representations $\mathcal{D}_l$ ($l = 0, 1, 2, ...$) of dimension $2l + 1$. Tensor representations of the rotation group are, in general, not irreducible. Each tensor representation $Q \mapsto Q^{\otimes r}|Z$ can be decomposed as a direct sum of subrepresentations, each of which is equivalent to some $\mathcal{D}_l$:

$$Z = n_0\mathcal{D}_0 + n_1\mathcal{D}_1 + \cdots + n_r\mathcal{D}_r, \tag{3}$$

where n_k is the multiplicity of $\mathcal{D}_k$ in the decomposition. When $Z = V^r$, we always have $n_r = 1$ in the decomposition formula. When Z is a proper subspace of V^r, some n_k's in Eq. (3) may be equal to zero, but we must have $\dim Z = \sum_{k=0}^{r} n_k(2k+1)$. For example, we have

$$[[V^2]^2] = 2\mathcal{D}_0 + 2\mathcal{D}_2 + \mathcal{D}_4, \tag{4}$$

$$[V^2][[V^2]^2] = 4\mathcal{D}_0 + 2\mathcal{D}_1 + 7\mathcal{D}_2 + 3\mathcal{D}_3 + 4\mathcal{D}_4 + \mathcal{D}_5 + \mathcal{D}_6, \tag{5}$$

and $\dim[[V^2]^2] = 21$, $\dim[V^2][[V^2]^2] = 126$. Here a term such as $\mathcal{D}_6$ in Eq. (5) denotes a $2 \times 6 + 1 = 13$ dimensional subspace of $[V^2][[V^2]^2]$, over which the subrepresentation of

$Q \mapsto Q^{\otimes 6}$ is equivalent to the irreducible representation $\mathcal{D}_6$. Decomposition formulae such as Eqs. (4) and (5) above can be derived by computing the character of the tensor representation in question [15, 17] or by other methods [16].

A tensor $\mathbb{H} \in Z \subset V^r$ is isotropic if and only if it takes value in the subspace $n_0\mathcal{D}_0$, which is a direct sum of n_0 1-dimensional subspaces invariant under $Q^{\otimes r}$. Thus we can read from Eqs. (4) and (5) that isotropic elasticity and acoustoelastic tensors in $[[V^2]^2]$ and $[V^2][[V^2]^2]$ are specified by two and four material constants, respectively.

In what follows we shall refer to formula (3) as the decomposition of the tensor space Z into its irreducible parts.

2.2. Orientation measures

For brevity, henceforth we write $\mathcal{G}$ for the rotation group SO(3), which is a compact topological group. Let $C(\mathcal{G})$ be the space of continuous complex functions on $\mathcal{G}$. It is a Banach space under the supremum norm. The elements of $C(\mathcal{G})^*$, the dual space of $C(\mathcal{G})$, are the Radon measures on $\mathcal{G}$. For $f \in C(\mathcal{G})$ and $\mu \in C(\mathcal{G})^*$, we denote by $\langle \mu, f \rangle$ the complex number that results when μ is applied to f. Anticipating the applications that we shall investigate, we call positive Radon measures $\wp$ with $\wp(\mathcal{G}) = 1$ orientation measures, and we denote by $\mathcal{M}(\mathcal{G})$ the set of orientation measures on $\mathcal{G}$. Under the weak* topology, $\mathcal{M}(\mathcal{G})$ is compact in $C(\mathcal{G})^*$ (cf. [18], p. 19).

For $Q \in \mathcal{G}$, the orientation measure δ_Q defined by

$$\langle \delta_Q, f \rangle = f(Q) \qquad \text{for each } f \in C(\mathcal{G})$$

is called the Dirac measure concentrated at Q. Discrete orientation measures are finite linear combinations of Dirac measures $\sum_i a_i \delta_{Q_i}$, where $a_i > 0$ for each i and $\sum_i a_i = 1$.

For orientation measures $\wp$ and a fixed $\mathbb{H}^o \in Z \subset V^r$, we consider (cf. Eq. (1))

$$\overline{\mathbb{H}}(\wp) = \int_{\mathcal{G}} R^{\otimes r} \mathbb{H}^o d\wp(R). \tag{6}$$

When the orientation measure $\wp$ is absolutely continuous with respect to the Haar measure $\wp_H$ (with $\wp_H(\mathcal{G}) = 1$), the Radon-Nikodym derivative $d\wp/d\wp_H$ is well defined. Following common practice, we call

$$w = \frac{1}{8\pi^2} \frac{d\wp}{d\wp_H} \tag{7}$$

the orientation distribution function (ODF), and we may recast Eq. (6) in terms of the ODF as

$$\overline{\mathbb{H}}(w) = 8\pi^2 \int_{\mathcal{G}} R^{\otimes r} \mathbb{H}^o w(R) d\wp_H(R). \tag{8}$$

If w is square integrable on $\mathcal{G}$ with respect to $\wp_H$, we may choose a spatial Cartesian coordinate system and expand w in an infinite series as follows:

$$w(R(\psi, \theta, \phi)) = \frac{1}{8\pi^2} + \sum_{l=1}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} c^l_{mn} D^l_{mn}(R(\psi, \theta, \phi)), \tag{9}$$

$$c^l_{mn} = (-1)^{m+n} \overline{c^l_{\bar{m}\bar{n}}}. \tag{10}$$

Here D^l_{mn} are the Wigner D-functions [19, 20]; (ψ, θ, ϕ) are the Euler angles [11] corresponding to the rotation R; $\overline{z}$ denotes the complex conjugate of the complex number z, and $\bar{m} = -m$. We call the expansion coefficients

$$c^l_{mn} = \frac{2l+1}{8\pi^2} \int_{\mathcal{G}} \overline{D^l_{mn}(R)} d\wp(R) \tag{11}$$

the texture coefficients; they are related to Roe's [11] coefficients W_{lmn} by the formula

$$W_{lmn} = (-1)^{m-n} \sqrt{\frac{2}{2l+1}}\, c^l_{mn}.$$

Let $\mathcal{M}_2(\mathcal{G})$ be the set of orientation measures which are absolutely continuous and have their corresponding ODF square integrable. Under the weak* topology, $\mathcal{M}_2(\mathcal{G})$ is dense in $\mathcal{M}(\mathcal{G})$, because discrete orientation measures lie (see, e.g. [21]) in the weak* closure of $\mathcal{M}_2(\mathcal{G})$ and they are dense in $\mathcal{M}(\mathcal{G})$ (see [18], p. 27).

For any sequence ${}^{(k)}w$ of square-integrable ODF's whose corresponding orientation measures ${}^{(k)}\wp$ converge weakly* to the Dirac measure δ_Q, by Eq. (11) their texture coefficients ${}^{(k)}c^l_{mn}$ converge to

$$c^l_{mn} = \frac{2l+1}{8\pi^2} \overline{D^l_{mn}(Q(\psi, \theta, \phi))}. \tag{12}$$

We call the c^l_{mn}'s given by Eq. (12) the texture coefficients pertaining to the Dirac measure δ_Q. Likewise, we associate a unique set of texture coefficients c^l_{mn} to each orientation measure $\wp$. Thus the texture coefficients c^l_{mn}, originally defined on $\mathcal{M}_2(\mathcal{G})$ by Eq. (11), are extended by continuity to become weakly* continuous functions on $\mathcal{M}(\mathcal{G})$.

Now consider an aggregate $\mathcal{A}$ which consists of a single crystallite $\mathcal{B}$ with crystal symmetry specified by a point group $\mathcal{G}_{\rm cr}$ which is a subgroup of the rotation group $\mathcal{G}$. Let $N_{\rm cr}$ be the order of $\mathcal{G}_{\rm cr}$, and let $\check{Q}_k$ ($k = 1, \ldots, N_{\rm cr}$) be the elements of $\mathcal{G}_{\rm cr}$. Suppose $\mathcal{B}$ assumes an orientation specified by the rotation R_0. The orientation measure of $\mathcal{A}$ is given by

$$\wp = \frac{1}{N_{\rm cr}} \sum_{k=1}^{N_{\rm cr}} \delta_k,$$

where δ_k is the Dirac measure concentrated at $R_0 \check{Q}_k$. The texture coefficients of $\mathcal{A}$ are then given by

$$c^l_{mn} = \frac{2l+1}{8\pi^2} \cdot \frac{1}{N_{\rm cr}} \cdot \sum_{k=1}^{N_{\rm cr}} \overline{D^l_{mn}(R_0 \check{Q}_k)}. \tag{13}$$

Let $\mathcal{G}^{(1)}$ be a finite subgroup of $\mathcal{G}$ with elements $Q^{(1)}_j$, $j = 1, \ldots, N_1$, where N_1 is the order of $\mathcal{G}^{(1)}$. Let $\mathcal{A}^{(1)}$ be an aggregate of N_1 crystallites $\mathcal{B}_j$ of equal volume, which have crystal symmetry $\mathcal{G}_{\rm cr}$ and orientations specified by $Q^{(1)}_j R_0$. The texture coefficients of $\mathcal{A}^{(1)}$ are:

$$c^l_{mn} = \frac{2l+1}{8\pi^2} \cdot \frac{1}{N_1} \cdot \frac{1}{N_{\rm cr}} \cdot \sum_{j=1}^{N_1} \sum_{k=1}^{N_{\rm cr}} \overline{D^l_{mn}(Q^{(1)}_j R_0 \check{Q}_k)}. \tag{14}$$

If the entire aggregate $\mathcal{A}^{(1)}$ is rotated by R_1, the rotated aggregate $\mathcal{A}_R^{(1)}$ will have texture coefficients

$$c_{mn}^l = \frac{2l+1}{8\pi^2} \cdot \frac{1}{N_1} \cdot \frac{1}{N_{\rm cr}} \cdot \sum_{j=1}^{N_1} \sum_{k=1}^{N_{\rm cr}} \overline{D_{mn}^l(R_1 Q_j^{(1)} R_0 \check{Q}_k)}. \tag{15}$$

Let $\mathcal{G}^{(2)}$ be a finite subgroup of $\mathcal{G}$ with elements $Q_i^{(2)}$, $i = 1, ..., N_2$, where N_2 is the order of $\mathcal{G}^{(2)}$. Let $\mathcal{A}^{(2)}$ be the aggregate of $N_1 \times N_2$ crystallites formed by replacing each crystallite $\mathcal{B}_j$ in the aggregate $\mathcal{A}_R^{(1)}$, whose orientation is $R_1 Q_j^{(1)} R_0$, with N_2 copies whose orientations are $Q_i^{(2)} R_1 Q_j^{(1)} R_0$ ($i = 1, ..., N_2$). The texture coefficients of aggregate $\mathcal{A}^{(2)}$ are:

$$c_{mn}^l = \frac{2l+1}{8\pi^2} \cdot \frac{1}{N_2} \cdot \frac{1}{N_1} \cdot \frac{1}{N_{\rm cr}} \cdot \sum_{i=1}^{N_2} \sum_{j=1}^{N_1} \sum_{k=1}^{N_{\rm cr}} \overline{D_{mn}^l(Q_i^{(2)} R_1 Q_j^{(1)} R_0 \check{Q}_k)}. \tag{16}$$

Let $\mathcal{G}_{\rm cr} = \mathcal{G}^{(0)}$, where $\mathcal{G}^{(0)} \subset \mathcal{G}$ is a specific point group. We call $\mathcal{A}^{(1)}$, and $\mathcal{A}^{(2)}$ aggregates of type $\mathcal{G}^{(1)} R_0 \mathcal{G}^{(0)}$, and $\mathcal{G}^{(2)} R_1 \mathcal{G}^{(1)} R_0 \mathcal{G}^{(0)}$, respectively. (We shall take aggregate $\mathcal{A}_R^{(1)}$ to be of the same type as that of $\mathcal{A}^{(1)}$.) In general, for $p \geq 1$, for a set of rotations $R_0, ..., R_{p-1}$, and finite subgroups $\mathcal{G}^{(1)}, ..., \mathcal{G}^{(p)}$ of the rotation group $\mathcal{G}$, we can easily write down the formula for the texture coefficients c_{mn}^l that pertain to the aggregate of type $\mathcal{G}^{(p)} R_{p-1} \mathcal{G}^{(p-1)} ... \mathcal{G}^{(1)} R_0 \mathcal{G}^{(0)}$, which consists of $N_p \times N_{p-1} \times \cdots \times N_1$ crystallites of equal volume and with $\mathcal{G}_{\rm cr} = \mathcal{G}^{(0)}$, namely:

$$c_{mn}^l = \frac{2l+1}{8\pi^2} \cdot \frac{1}{N_p} \cdot ... \cdot \frac{1}{N_1} \cdot \frac{1}{N_0} \cdot \sum_{i_p=1}^{N_p} ... \sum_{i_1=1}^{N_1} \sum_{i_0=1}^{N_0} \overline{D_{mn}^l(Q_{i_p}^{(p)} R_{p-1} \cdots Q_{i_1}^{(1)} R_0 Q_{i_0}^{(0)})}, \tag{17}$$

where the order and elements of $\mathcal{G}^{(0)}$ are denoted by N_0 and $Q_{i_0}^{(0)}$ ($i_0 = 1, ..., N_0$), respectively.

3. The ODF method

Let $w_{\rm iso} = 1/(8\pi^2)$, the ODF when all texture coefficients are zero. Let $m = 8\pi^2 \wp_H$, and let $L^2(\mathcal{G}, m)$ be the space of complex functions on $\mathcal{G}$ which are square integrable with respect to the measure m. Let

$$\mathcal{H}_0 = \{f \in L^2(\mathcal{G}, m) : \int_{\mathcal{G}} f \, dm = 0\}, \tag{18}$$

$$\mathcal{H} = \{w \in L^2(\mathcal{G}, m) : w = w_{\rm iso} + f, \text{ where } f \in \mathcal{H}_0\}. \tag{19}$$

All orientation distribution functions w fall in $\mathcal{H}$.

Let w be the ODF which characterizes the crystallographic texture of a polycrystalline aggregate $\mathcal{A}$. After $\mathcal{A}$ undergoes a rotation Q, its texture is described by a new ODF $\mathcal{T}_Q w$, which is related to w, the ODF before rotation, by the formula

$$\mathcal{T}_Q w(R) = w(Q^T R) \tag{20}$$

for each rotation R.

The tensor function $\overline{\mathbb{H}} : \mathcal{M}(\mathcal{G}) \longrightarrow V^r$, as defined in Eq. (6) by orientational averaging, is weakly* continuous. When restricted to $\mathcal{M}_2(\mathcal{G})$, the function $\overline{\mathbb{H}}(\cdot)$ can be taken as a function of the ODF. This function is defined by Eq. (8), which makes sense for any argument f in $L^2(\mathcal{G}, m)$. As is apparent from Eq. (8), the extended function $f \mapsto \overline{\mathbb{H}}(f)$ is strongly continuous on $L^2(\mathcal{G}, m)$. Substituting Eq. (9) into Eq. (8), we observe that

$$\overline{\mathbb{H}}(w) = \overline{\mathbb{H}}_{\text{iso}} + \overline{\mathbb{H}}'[w - w_{\text{iso}}], \tag{21}$$

where

$$\overline{\mathbb{H}}_{\text{iso}} = \int_{\mathcal{G}} R^{\otimes r} \mathbb{H}^o d\wp_H(R)$$

is the isotropic part of $\overline{\mathbb{H}}$, and

$$\overline{\mathbb{H}}'[w - w_{\text{iso}}] = 8\pi^2 \sum_{l=1}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} c^l_{mn} \int_{\mathcal{G}} R^{\otimes r} \mathbb{H}^o D^l_{mn}(R) d\wp_H(R),$$

the anisotropic part, is linear and strongly continuous on $\mathcal{H}_0$. From the invariance of the Haar measure $\wp_H$, we observe immediately that $\overline{\mathbb{H}}'$ satisfies the constraint

$$\overline{\mathbb{H}}'[\mathcal{T}_Q w - w_{\text{iso}}] = Q^{\otimes r} \left(\overline{\mathbb{H}}'[w - w_{\text{iso}}]\right) \tag{22}$$

for each rotation Q.

Tensor functions defined by orientational averaging are prime examples of the class (*) of material tensors that we study in this paper. We formalize this class with a definition.

DEFINITION 2. *Let Z be a subspace of V^r which is invariant under $Q^{\otimes r}$ for each rotation Q. We say that a tensor function $\mathbb{B} : \mathcal{M}(\mathcal{G}) \longrightarrow Z$ is of class (*) if*

(i) $\mathbb{B}$ *is weakly* continuous;*

(ii) when restricted to $\mathcal{M}_2(\mathcal{G})$,

$$\mathbb{B}(w) = \mathbb{B}_{\text{iso}} + \mathbb{B}'[w - w_{\text{iso}}], \tag{23}$$

where $\mathbb{B}_{\text{iso}}$ is isotropic and $\mathbb{B}'[\cdot]$ is linear and strongly continuous on $\mathcal{H}_0$;

(iii) $\mathbb{B}[\cdot]$ observes the constraint

$$\mathbb{B}'[\mathcal{T}_Q w - w_{\text{iso}}] = Q^{\otimes r} \left(\mathbb{B}'[w - w_{\text{iso}}]\right) \tag{24}$$

for each rotation Q.

Besides tensors defined by orientational averaging, class (*) includes material tensors pertaining to "weakly textured" polycrystals [8, 9]. Henceforth we shall consider only tensor functions of class (*).

Let $\mathbb{B} : \mathcal{M}(\mathcal{G}) \longrightarrow Z \subset V^r$ be a tensor function of class (*). In our method for designing aggregates with an isotropic $\mathbb{B}$, the following observation is instrumental:

(#) Let $Z = n_0\mathcal{D}_0 + n_1\mathcal{D}_1 + \cdots + n_r\mathcal{D}_r$ be the decomposition of the tensor space Z into its irreducible parts. Let $\mathbb{B}(\wp) = \mathbb{B}_0(\wp) + \mathbb{B}_1(\wp) + \mathbb{B}_2(\wp) + \ldots + \mathbb{B}_r(\wp)$, where $\mathbb{B}_k(\cdot)$ ($k = 0, 1, \ldots, r$) takes values in the $n_k \times (2k+1)$ dimensional subspace $n_k\mathcal{D}_k$ of Z. For $k \geq 1$, the components of $\mathbb{B}_k(\wp)$ are linear combinations of only those texture coefficients c^l_{mn} with $l = k$.

Observation (#) is an immediate corollary of a theorem due to Man [13].

REMARK 1. The tensor $\mathbb{B}(\wp)$ is isotropic if and only if $\mathbb{B}_k(\wp) = 0$ for $k = 1, 2, ..., r$. Hence, to design an aggregate with an isotropic $\mathbb{B}$, it suffices to find an orientation measure $\wp$ which has its $c^l_{mn} = 0$ for those $1 \leq l \leq r$ with $n_l \neq 0$ in the decomposition formula for Z above.

REMARK 2. Let $\mathcal{G}^{(0)}$ and $\mathcal{G}^{(p)}$ be finite rotation groups that satisfy the crystallographic restriction, and let $\mathcal{G}^{(1)}, \ldots, \mathcal{G}^{(p-1)}$ be finite rotation groups. Let $\mathcal{A}$ and $\hat{\mathcal{A}}$ be aggregates of type $\mathcal{G}^{(p)} R_{p-1} \mathcal{G}^{(p-1)} ... \mathcal{G}^{(1)} R_0 \mathcal{G}^{(0)}$ and type $\mathcal{G}^{(0)} R_0^T\ \mathcal{G}^{(1)} ... \mathcal{G}^{(p-1)} R^T_{p-1} \mathcal{G}^{(p)}$, respectively, and let c^l_{mn} and $\hat{c}^l_{mn}$ be their texture coefficients. Since $D^l_{mn}(R^T) = \overline{D^l_{nm}(R)}$ for each rotation R, we see that $\hat{c}^l_{mn} = \overline{c^l_{nm}}$. Hence, if all $c^l_{mn} = 0$ for a specific set of l's, then all $\hat{c}^l_{mn} = 0$ for the same set of l's, and vice versa. Thus, if we can find an aggregate of type $\mathcal{G}^{(p)} R_{p-1} \mathcal{G}^{(p-1)} ... \mathcal{G}^{(1)} R_0\, \mathcal{G}^{(0)}$ which has an isotropic $\mathbb{B}$, we obtain at once another aggregate of type $\mathcal{G}^{(0)} R_0^T\ \mathcal{G}^{(1)} ... \mathcal{G}^{(p-1)} R^T_{p-1} \mathcal{G}^{(p)}$ which has an isotropic $\mathbb{B}$.

By Remark 1, the problem of designing aggregates with their elasticity tensors isotropic reduces to that of designing aggregates with all their c^2_{mn}'s and c^4_{mn}'s zero. By the same token, an aggregate with all its $c^l_{mn} = 0$ for $1 \leq l \leq 6$ has both its elasticity and acoustoelastic tensors isotropic. In any case, to design an aggregate which has a finite set of specific material tensors isotropic, we just need to determine an arrangements of grains so that the resulting aggregate has all its $c^l_{mn} = 0$ for an appropriate finite set of l's. Let us now proceed to examine this problem.

With the original formulation of the problem of Bertram et al. [1, 2] in mind, here we seek only aggregates whose constituting crystallites all have equal volume. For simplicity, whenever no confusion should arise, we shall simply say "identical grains" or just "grains" when we really mean crystallites of the same material that have equal volume. In fact, all solutions reported in Sections 4 and 5 below are aggregates of "identical grains".

Consider a polycrystalline aggregate $\mathcal{A}$, which undergoes a rotation Q. Let c^l_{mn} and $\tilde{c}^l_{mn}$ be the texture coefficients of the aggregate before and after the rotation. These two sets of texture coefficients are related by the formula [8, 11]

$$\tilde{c}^l_{mn} = \sum_{p=-l}^{l} c^l_{pn} D^l_{pm}(Q^{-1}). \tag{25}$$

For a fixed l and n, if $c^l_{mn} = 0$ for all $-l \leq m \leq l$, then $\tilde{c}^l_{mn} = 0$ for all $-l \leq m \leq l$, irrespective of the rotation Q. This observation suggests a procedure for constructing an aggregate of crystallites with $\mathcal{G}_{\text{cr}} = \mathcal{G}^{(0)}$ which has all its $c^l_{mn} = 0$ for a specific finite set of l's (say, for $l = l_1, ..., l_a$):

1. For $l = l_1$ and an n_i between $-l_1$ and l_1, find an aggregate $\mathcal{A}^{(1)}$ of type $\mathcal{G}^{(1)} R_0 \mathcal{G}^{(0)}$ (see Section 2.2 above) which has $c^{l_1}_{mn_i} = 0$ for $-l_1 \leq m \leq l_1$. The job here is to seek an appropriate rotation R_0 and a finite rotation group $\mathcal{G}^{(1)}$ which meet the requirement. The aggregate $\mathcal{A}^{(1)}$ has $\mathcal{G}^{(1)}$ and $\mathcal{G}^{(0)}$ as its group of texture symmetry and crystal symmetry, respectively. This knowledge will facilitate the search for an appropriate R_0 and $\mathcal{G}^{(1)}$, as we shall see from the specific examples in the next two sections.
2. Depending on the specific l_1 and $\mathcal{G}^{(0)}$, the aggregate $\mathcal{A}^{(1)}$ may already have its $c^{l_1}_{mn} = 0$ for all $-l_1 \leq m \leq l_1$ and $-l_1 \leq n \leq l_1$. If that is the case, for $l = l_2$ and an

n_i between $-l_2$ and l_2, find an aggregate $\mathcal{A}^{(2)}$ of type $\mathcal{G}^{(2)}R_1\mathcal{G}^{(1)}R_0\mathcal{G}^{(0)}$ which has $c^{l_2}_{mn_i} = 0$ for $-l_2 \le m \le l_2$. Since R_0 and $\mathcal{G}^{(1)}$ have already been determined, the task here is to find an appropriate rotation R_1 and a suitable finite rotation group $\mathcal{G}^{(2)}$. The aggregate $\mathcal{A}^{(2)}$ has $\mathcal{G}^{(2)}$ and $\mathcal{G}^{(0)}$ as its group of texture symmetry and crystal symmetry, respectively. Because of the transformation formula (25), aggregate $\mathcal{A}^{(2)}$ still has its $c^{l_1}_{mn} = 0$, irrespective of our choice of R_1 and $\mathcal{G}^{(2)}$ which renders the texture coefficients $c^{l_2}_{mn_i}$ of $\mathcal{A}^{(2)}$ null for all $-l_2 \le m \le l_2$. If there is an $n_j \ne n_i$ such that $c^{l_1}_{mn_j} \ne 0$ for some m, find an aggregate $\mathcal{A}^{(2)}$ of type $\mathcal{G}^{(2)}R_1\mathcal{G}^{(1)}R_0\mathcal{G}^{(0)}$ such that $c^{l_1}_{mn_j} = 0$ for all $-l_1 \le m \le l_1$.

3. Repeat the preceding procedure iteratively to find an aggregate of type $\mathcal{G}^{(p)}R_{p-1}\mathcal{G}^{(p-1)}$ $\ldots\mathcal{G}^{(1)}R_0\mathcal{G}^{(0)}$ which has all its $c^l_{mn} = 0$ for $l = l_1, \ldots, l_a$.

We shall work out a few concrete examples in the next two sections to illustrate the procedure described above.

4. Example: elasticity tensor

As our first example, let us consider the elasticity tensor $\mathbb{C}$. By decomposition formula (3) and observation (#), if we wish to design an aggregate with an isotropic elasticity tensor of class (*), we need only to find an aggregate whose c^2_{mn} and c^4_{mn} coefficients are zero. We begin our discussion by revisiting the problem solved by Bertram et al. [1, 2], namely, that of cubic grains.

In what follows we always assume that a fixed spatial Cartesian coordinate system has been chosen. We write e_1, e_2, and e_3 for the orthonormal basis vectors that define this coordinate system. For a unit vector e and an angle $\omega \in [0, \pi]$, we denote by $R(e, \omega)$ the rotation about e by angle ω. All angles given below are in radians.

4.1. Cubic grains

Here $\mathcal{G}_{\rm cr} = O$. We choose a reference crystallite which has its three four-fold axes of cubic symmetry in line with the three spatial coordinate axes. This is tantamount to choosing $R(e_1, \pi/2)$, $R(e_2, \pi/2)$, and $R(e_3, \pi/2)$ to be the generators of the group O of crystal symmetry. With this choice of reference, the texture coefficients of any aggregate of cubic grains satisfy [10, 11] the equation

(26)
$$c^l_{mn} = \sum_{p=-l}^{l} c^l_{mp} D^l_{np}(Q),$$

for each of the 24 rotations Q in the symmetry group of the reference crystallite. As a result, any aggregate of cubic grains has [22] their c^2_{mn} coefficients all zero. Moreover, of the c^4_{mn} coefficients, only one coefficient is independent for each fixed m ($-4 \le m \le 4$), and c^4_{m0} ($-4 \le m \le 4$) may be chosen as the independent coefficients. An aggregate of cubic grains with $c^4_{m0} = 0$ for each m has all its c^2_{mn} and c^4_{mn} coefficients vanish and thence has an isotropic $\mathbb{C}$.

For an aggregate of one grain, there are nine equations (i.e., $c^4_{\bar{4}0}(R_0) = 0$, $c^4_{\bar{3}0}(R_0) = 0$, $c^4_{\bar{2}0}(R_0) = 0, \ldots, c^4_{20}(R_0) = 0$, $c^4_{30}(R_0) = 0$, $c^4_{40}(R_0) = 0$, where each texture coefficient is in the form of Eq. (13)) to be solved for one orientation $R_0(\psi_0, \theta_0, \phi_0)$. Clearly there need not be a solution. In fact, thanks to the work of Bertram et al. [1], we already know that this system of nine equations has no solution for R_0. By adding additional identical grains in specific orientations dictated by a group $\mathcal{G}^{(1)}$ of texture symmetry, we can place additional restrictions on the texture coefficients and reduce the number of equations which must be satisfied.

Suppose we add three identical cubic grains and arrange them so that the aggregate has orthorhombic texture symmetry with the coordinate axes being the axes of two-fold rotational symmetry (i.e., $\mathcal{G}^{(1)} = D_2$ with $R(e_2, \pi)$ and $R(e_3, \pi)$ as generators). The texture coefficients must be calculated as in Eq. (14) but there are fewer independent coefficients. For $Q \in D_2$, Eq. (25) implies that

$$c^l_{mn} = \sum_{p=-l}^{l} c^l_{mp} D^l_{np}(Q^{-1}) \tag{27}$$

holds. By considering $Q(\psi, \theta, \phi) = (0, \pi, 0)$ and $Q(\psi, \theta, \phi) = (0, 0, \pi)$, we determine that $c^l_{mn} = 0$ if m is odd, and $c^l_{\bar{m}n} = (-1)^l c^l_{mn}$ if m is even. Hence, under this texture symmetry/crystal symmetry combination, the only independent c^4_{m0} coefficients can be chosen to be c^4_{00}, c^4_{20}, and c^4_{40}, and by making these coefficients zero, all c^4_{mn} vanish.

The result is a system of three equations:

$$c^4_{00}(R_0) = 0, \qquad c^4_{20}(R_0) = 0, \qquad c^4_{40}(R_0) = 0, \tag{28}$$

where each texture coefficient is of the form given in Eq. (14). Since R_0 is parametrized by Euler angles, the equations need only be solved for $(\psi_0, \theta_0, \phi_0)$. We used the computer algebra system Maple to find solutions to the three simultaneous equations. Because of the D_2 texture symmetry and O crystal symmetry, two solutions R_0 and $R_0^\#$ of system (28) describe the same arrangement of grains if

$$R_0^\# = \widetilde{Q} R_0 \check{Q}$$

for some $\widetilde{Q} \in D_2$ and $\check{Q} \in O$. Surely we should regard such an R_0 and $R_0^\#$ as equivalent solutions. Since $|D_2| = 4$, $|O| = 24$, and D_2 is a subgroup of O, given a solution R_0 there will be 96, 48, or 24 solutions equivalent to it if R_0 commutes with none, one, or both of the generators of D_2. From our Maple solutions of (28), we identified the following four, which are not equivalent in the preceding sense:

$$R_0^{(1)}(\psi_0, \theta_0, \phi_0) = (0.59549275, 0.52174397, 0.59549275), \tag{29}$$

$$R_0^{(2)}(\psi_0, \theta_0, \phi_0) = (2.16628908, 0.52174397, 0.59549275), \tag{30}$$

$$R_0^{(3)}(\psi_0, \theta_0, \phi_0) = (0.97530358, 0.52174397, 0.97530358), \tag{31}$$

$$R_0^{(4)}(\psi_0, \theta_0, \phi_0) = (2.54609990, 0.52174397, 0.97530358), \tag{32}$$

where the angles are given in radians. The preceding solutions are clearly related by the equations

$$R_0^{(2)} = R(e_3, \pi/2) R_0^{(1)}, \qquad R_0^{(4)} = R(e_3, \pi/2) R_0^{(3)}. \tag{33}$$

Solution $R_0^{(1)}$ is none other than the 4-grain solution found by Bertram et al. [1, 2].

Let $\mathcal{A}_i$ ($i = 1, 2, 3, 4$) be the aggregate described by solution $R_0^{(i)}$. Since

$$R(e_3, \pi/2) D_2 = D_2 R(e_3, \pi/2),$$

we observe from (33) that $\mathcal{A}_2$ and $\mathcal{A}_4$ result if we rotate aggregates $\mathcal{A}_1$ and $\mathcal{A}_3$ by $R(e_3, \pi/2)$, respectively. We take aggregates $\mathcal{A}_2$ and $\mathcal{A}_4$ to be of the same type as $\mathcal{A}_1$ and $\mathcal{A}_3$, respectively.

For brevity, let us simply write R_0 for $R_0^{(1)}$. Then aggregate $\mathcal{A}_1$ is of type $D_2 R_0 O$. If we write $R_0(\psi_0, \theta_0, \phi_0) = (\alpha, \beta, \alpha)$, then $R_0^{(3)}(\psi_0, \theta_0, \phi_0) = (\pi/2 - \alpha, \beta, \pi/2 - \alpha)$. Construct an aggregate $\widetilde{\mathcal{A}}$ by rearranging the grains in $\mathcal{A}_1$ so that R_0 is replaced by R_0^T, which has Euler angles $(\pi - \alpha, \beta, \pi - \alpha)$ and is equivalent to $(\pi - \alpha, \beta, \pi/2 - \alpha)$ for a $D_2 R_0^T O$ aggregate. If we rotate $\widetilde{\mathcal{A}}$ by $R(e_3, -\pi/2)$, we obtain aggregate $\mathcal{A}_3$ because $R(e_3, -\pi/2) D_2 = D_2 R(e_3, -\pi/2)$. Hence $\mathcal{A}_3$ is of type $D_2 R_0^T O$.

4.2. Grains of other crystal symmetries

In Eq. (29) we obtain an aggregate $\mathcal{A}^{(1)}$ of type $D_2 R_0 O$, which has its elasticity tensor $\mathbb{C}$ isotropic. From this solution we can construct, for crystallites of any $\mathcal{G}_{\rm cr} \subset \mathcal{G}$, an aggregate with an isotropic $\mathbb{C}$.

The method is as follows: Let R_1 be any rotation and $\mathcal{G}^{(2)}$ be any finite subgroup of $\mathcal{G}$ which satisfies the crystallographic restriction. If we rotate the aggregate $\mathcal{A}^{(1)}$ by R_1, the rotated aggregate $\mathcal{A}_R^{(1)}$ still has its $\mathbb{C}$ isotropic. Now append grains to $\mathcal{A}_R^{(1)}$ to obtain an aggregate of type $\mathcal{G}^{(2)} R_1 D_2 R_0 O$, which is simply an assembly of N_2 (the order of $\mathcal{G}^{(2)}$) rotated copies of $\mathcal{A}_R^{(1)}$. Clearly the new assembly has an isotropic $\mathbb{C}$. By Remark 2, we conclude that the aggregate of type $O R_0^T D_2 R_1^T \mathcal{G}^{(2)}$, which consists of $24 \times 4 = 96$ grains with $\mathcal{G}_{\rm cr} = \mathcal{G}^{(2)}$, also has an isotropic $\mathbb{C}$. In other words, for crystallites with its $\mathcal{G}_{\rm cr}$ being a finite rotation group, including triclinic crystallites with $\mathcal{G}_{\rm cr} = C_1$, we can always design an aggregate with 96 identical grains which has an isotropic elasticity tensor.

The appearance of an arbitrary rotation R_1 in the preceding scheme suggests that this recipe generally will not lead to a solution with the least possible number of grains. Indeed for many crystal symmetries we can achieve our goal using less grains. Let us now present one other solution for each $\mathcal{G}_{\rm cr} \subset \mathcal{G}$ other than C_1.

$\underline{\mathcal{G}_{\rm cr} = D_2, D_4, D_6}$

By Remark 2, $O R_0^T D_2$ is a solution with 24 orthorhombic grains. Moreover, if $\mathcal{G}^{(1)}$ contains D_2 as a subgroup, then the 24-grain aggregate of type $O R_0^T\ \mathcal{G}^{(1)}$ also has an isotropic $\mathbb{C}$. Indeed, let $q = |\mathcal{G}^{(1)}|/|D_2|$ and

$$\mathcal{G}^{(1)} = \bigcup_{i=1}^{q} g_i D_2, \qquad \text{(disjoint union)} \tag{34}$$

where $\{g_i : i = 1, ..., q\}$ is a set of left coset representatives of D_2 in $\mathcal{G}^{(1)}$. An aggregate of type $\mathcal{G}^{(1)} R_0 O$ can be taken as a "super-aggregate" of q rotated copies of the aggregate of type $D_2 R_0 O$, where g_i $(i = 1, ..., q)$ describe the rotations in question. Since each rotated copy has an isotropic $\mathbb{C}$, so does the super-aggregate. It follows from Remark 2 that an aggregate of type $O R_0^T \mathcal{G}^{(1)}$ also has an isotropic $\mathbb{C}$.

The same argument in fact proves a general assertion, which we put as the next remark.

REMARK 3. Let $\mathcal{G}_a$ and $\mathcal{G}_b$ be point groups such that $\mathcal{G}_a \subset \mathcal{G}_b \subset \mathcal{G} = \mathrm{SO}(3)$. If an aggregate of type $\mathcal{G}^{(p)} R_{p-1} \mathcal{G}^{(p-1)} ... \mathcal{G}^{(1)} R_0 \mathcal{G}_a$ has its material tensors $\mathbb{H}^{(1)}, ..., \mathbb{H}^{(p)}$ isotropic, so does an aggregate of type $\mathcal{G}^{(p)} R_{p-1} \mathcal{G}^{(p-1)} ... \mathcal{G}^{(1)} R_0 \mathcal{G}_b$.

By the preceding remark, cubic aggregates of 24 tetragonal and hexagonal crystallites which are of type $OR_0^T D_4$ and $OR_0^T D_6$, respectively, have their elasticity tensor isotropic; here we take rotations $R(e_2, \pi)$ and $R(e_3, \pi/2)$ as the two generators of group D_4 and rotations $R(e_2, \pi)$ and $R(e_3, \pi/3)$ as the two generators of group D_6.

$\mathcal{G}_{\rm cr} = C_2, C_4, C_6$

Let $C_2^{(1)} = \{I, R(e_3, \pi)\}$ and $C_2^{(2)} = \{I, R(e_2, \pi)\}$, where I is the identity in $\mathcal{G}$. The solution of type $D_2 R_0 O$ can be looked upon as of type $C_2^{(1)} I C_2^{(2)} R_0 O$. By Remark 2, we obtain a solution of type $OR_0^T C_2^{(2)} I C_2^{(1)}$, which consists of $24 \times 2 = 48$ C_2-grains of equal volume.

Let $R(e_3, \pi/2)$ and $R(e_3, \pi/3)$ be the generator of group C_4 and C_6, respectively. Since both C_4 and C_6 include $C_2^{(1)}$ as a subgroup, by Remark 3 we conclude that aggregates of type $OR_0^T C_2^{(2)} I C_4$ and $OR_0^T C_2^{(2)} I C_6$ are also solutions. These aggregates are made up of 48 C_4- and C_6-grains, respectively.

$\mathcal{G}_{\rm cr} = C_3$

First we present a solution of hexagonal grains which exhibits C_3 texture symmetry. To start with, we arrange an aggregate of 8 identical hexagonal grains so that it has tetragonal texture symmetry (i.e. $\mathcal{G}^{(1)} = D_4$, where $R(e_2, \pi)$ and $R(e_3, \pi/2)$ are taken as generators). Then, by determining the independent coefficients for $l = 4$ and solving the resulting equations with texture coefficients of form shown in Eq. (14), we find that the orientation

$$R_0(\psi_0, \theta_0, \phi_0) = (0.39269908,\ 1.22389959,\ 0) \tag{35}$$

generates an aggregate of type $D_4 R_0 D_6$ which has all its c^4_{mn} coefficients zero.

By placing three copies of this aggregate in such a way that the super-aggregate has C_3 texture (i.e. $\mathcal{G}^{(2)} = C_3$, with $R(e_3, 2\pi/3)$ as generator), we are able to determine that among the c^2_{mn} coefficients of the super-aggregate only the coefficient c^2_{00} is independent, and $c^2_{00} = 0$ renders all c^2_{mn} coefficients zero. Moreover, we find that

$$R_1(\psi_1, \theta_1, \phi_1) = (0,\ 0.95531662,\ 0)$$

is a solution of $c^2_{00} = 0$, where the texture coefficient is of form Eq. (16) with R_0 given by Eq. (35). Thus we obtain an aggregate of type $C_3 R_1 D_4 R_0 D_6$, which has an isotropic elasticity tensor $\mathbb{C}$.

By Remark 2, aggregates of type $D_6 R_0^T D_4 R_1^T C_3$, which consist of $12 \times 8 = 96$ C_3-grains of equal volume, have their elasticity tensor isotropic.

$\mathcal{G}_{\rm cr} = D_3$

We found an arrangement of 24 D_3-grains, for which the elasticity tensor $\mathbb{C}$ of the aggregate is isotropic. The arrangement is of type $OR_0 D_3$, where

$$R_0(\psi_0, \theta_0, \phi_0) = (0.55357436,\ \pi/2,\ 0).$$

$\mathcal{G}_{cr} = T$

In paper [1] Bertram et al. have presented a solution of type $T R_0 O$, where

$$R_0(\psi_0, \theta_0, \phi_0) = (0.24002358,\ 2.67480609,\ 2.90156907). \tag{36}$$

Hence there is a solution of type $O R_0^T T$ with 24 tetrahedral grains. In fact, $R_0^T = R_0$ in this case.

In summary, we have presented at least one solution for each $\mathcal{G}_{cr}$ which is a finite rotation group that satisfies the crystallographic restriction. For each $\mathcal{G}_{cr}$, our best solution at present (where using a smaller number of grains means better) requires 4 grains for $\mathcal{G}_{cr} = O$; 24 grains for $\mathcal{G}_{cr} = D_2$, D_3, D_4, D_6, or T; 48 grains for $\mathcal{G}_{cr} = C_2, C_4$, or C_6; 96 grains for $\mathcal{G}_{cr} = C_1$, or C_3. Except for the case of cubic grains, where a proof was given by Bertram et al. [1], it remains unclear whether the solution we presented would be a minimal solution, i.e., one with the least possible number of identical grains for the $\mathcal{G}_{cr}$ in question. In fact, we believe that many of our present "best solutions" can be improved upon.

5. Example: acoustoelastic tensor

In a similar manner, it is possible to build textured aggregates which have isotropic tensors of higher order. As an example, here we seek designs which render the sixth-order acoustoelastic tensor $\mathbb{D}$ [5, 6] isotropic. A glance at decomposition formula (5) reveals that we should design aggregates with their c^l_{mn} coefficients all zero for $1 \le l \le 6$. A solution in this regard will not only have its acoustoelastic tensor $\mathbb{D}$ isotropic, but will also attain (cf. Section 2.1) isotropy for all its material tensors of order $l \le 6$, including the fourth-order elasticity tensor $\mathbb{C}$.

For all the finite rotation groups that appear below, we have already specified their generators in the preceding section. For groups of crystal symmetry, the generators help specify the orientation of the reference crystallite with respect to the chosen spatial Cartesian coordinate system.

5.1. Cubic grains

With our choice of reference crystallite and spatial coordinate system, the restrictions imposed by crystal symmetry (see Eq. (26)) dictate [10, 22] that any aggregate of cubic grains must have all their c^l_{mn} coefficients vanish for $l = 1, 2, 3, 5$. Hence we just need to worry about the c^4_{mn} and c^6_{mn} coefficients.

Consider an arrangement of 8 identical cubic grains so that the aggregate $\mathcal{A}^{(1)}$ has tetragonal texture symmetry (i.e. $\mathcal{G}_{cr} = O$ and $\mathcal{G}^{(1)} = D_4$). From the fact that Eqs. (26) and (27) should hold for $Q \in O$ and $Q \in D_4$, respectively, we observe that all the c^6_{mn} coefficients will vanish if c^6_{00} and c^6_{40} are null. Using Maple to solve the equations $c^6_{00}(R_0) = 0$ and $c^6_{40}(R_0) = 0$, where the texture coefficients are in the form of Eq. (14), we found that

$$R_0(\psi_0, \theta_0, \phi_0) = (0.08033115,\ 2.63923776,\ 0.99945255) \tag{37}$$

is an orientation which makes all the c^6_{mn} coefficients vanish for the aggregate $\mathcal{A}^{(1)}$ of type $D_4 R_0 O$.

Place 4 identical copies of this $\mathcal{A}^{(1)}$ aggregate so that the new super-aggregate $\mathcal{A}^{(2)}$ has orthorhombic texture symmetry D_2. Equation (25) reminds us that the c^6_{mn} coefficients of $\mathcal{A}^{(2)}$

vanish since all the c^6_{mn} coefficients of $\mathcal{A}^{(1)}$ are zero. Because of the D_2 texture symmetry, we only need to solve a system of three equations:

$$c^4_{00}(R_1) = 0, \qquad c^4_{20}(R_1) = 0, \qquad c^4_{40}(R_1) = 0, \tag{38}$$

where each texture coefficient is of the form given in Eq. (16).

Using Maple, we found a solution

$$R_1(\psi_1, \theta_1, \phi_1) = (0.10523426, 0.47936161, 0.28647879). \tag{39}$$

Thus we have constructed an aggregate of type $D_2 R_1 D_4 R_0 O$ consisting of $4 \times 8 = 32$ identical cubic grains which has all its material tensors of order $l \leq 6$ isotropic.

5.2. Grains of other crystal symmetries

By the argument given in Section 4.2, we know that for any rotation R_2 and point group $\mathcal{G}^{(3)} \subset \mathcal{G}$, an aggregate $\mathcal{A}^{(3)}$ of type $O R_0^T D_4 R_1^T D_2 R_2^T \mathcal{G}^{(3)}$, where R_0 and R_1 are given by Eqs. (37) and (39), respectively, has all its material tensors of order $l \leq 6$ isotropic. Such an aggregate consists of $24 \times 8 \times 4 = 768$ identical grains of crystal symmetry $\mathcal{G}_{\rm cr} = \mathcal{G}^{(3)}$.

For most crystal symmetries, we expect that we can achieve the same goal with a smaller number of grains. For instance, by Remark 2 and 3, aggregates of types $O R_0^T D_4 R_1^T D_2$, $O R_0^T D_4 R_1^T D_4$, and $O R_0^T D_4 R_1^T D_6$, where R_0 and R_1 are given by Eqs. (37) and (39), respectively, have all their material tensors of order $l \leq 6$ isotropic. These aggregates are made up of $24 \times 8 = 192$ identical orthorhombic, tetragonal, and hexagonal grains, respectively.

Likewise, by treating an aggregate of type $D_2 R_1 D_4 R_0 O$ as of type $C_2^{(1)} I C_2^{(2)} R_1 D_4 R_0 O$, where $C_2^{(1)}$ and $C_2^{(2)}$ are defined in Sec. 4.2, we obtain a solution of type $O R_0^T D_4 R_1^T C_2^{(2)} I C_2^{(1)}$, which consists of $24 \times 8 \times 2 = 384$ C_2-grains of equal volume. By Remark 3, aggregates of type $O R_0^T D_4 R_1^T C_2^{(2)} I C_4$ and of type $O R_0^T D_4 R_1^T C_2^{(2)} I C_6$ are also solutions. These aggregates are made up of 384 C_4- and C_6-grains, respectively.

6. Discussion

The outlined method allows the construction of aggregates having isotropic tensors of various orders. So long as $\mathcal{G}_{\rm cr}$ is a finite subgroup of the rotation group $\mathcal{G}$, the specific crystal symmetry of the crystallites is of no concern. Indeed we have shown in Sections 4 and 5 that once a design of any type is found for an aggregate of identical grains which has a specific set of material tensors isotropic, it generates for each such $\mathcal{G}_{\rm cr}$ a solution which has the same set of tensors isotropic. Our ODF method can be easily implemented using any software which can solve (nonlinear) systems of equations.

But there are limitations. At each step, say the p-th, the method requires finding a rotation $R_{p-1}(\psi_{p-1}, \theta_{p-1}, \phi_{p-1})$ which satisfies a system of nonlinear equations $c^l_{mn}(R_{p-1}) = 0$, where c^l_{mn} is of the form (17), l and n are given, and m runs over those indices between $-l$ and l for which the texture coefficients c^l_{mn} are independent for aggregates with $\mathcal{G}^{(p)}$ as the group of texture symmetry. When the number of independent indices is bigger than three, there are more equations than the number of unknowns. While nothing can be said for sure because the equations are nonlinear, it is likely that the method would break down when that happens. To reduce the number of independent m's, we could take $\mathcal{G}^{(p)}$ to be a group of larger order. For example, for $\mathcal{G}^{(p)} = O$, the number of independent m's is not bigger than three when $l \leq 34$.

Of course, we hardly need to worry about tensors of order higher than 34 in practice. But taking $\mathcal{G}^{(p)} = O$ at every step is also impractical. The equations describing the c^l_{mn} coefficients quickly become unwieldy as l is increased or when the orders of the symmetry groups involved are large. In this case, it may be infeasible to find solutions even if they exist. Using $\mathcal{G}_{\rm cr}$ and $\mathcal{G}^{(p)}$ $(p \geq 1)$ of smaller orders will simplify the equations. A smaller $\mathcal{G}_{\rm cr}$, however, will increase the number of steps required because for each l there will be more (l, n) pairs for which the c^l_{mn} coefficients must be considered. A smaller $\mathcal{G}^{(p)}$ will increase the number of equations at the p-th step. Hence the method relies on finding a suitable combination of $\mathcal{G}_{\rm cr}$ and $\mathcal{G}^{(p)}$ $(p \geq 1)$ which produces solvable systems of equations at all the necessary steps that lead to the design of a suitable aggregate. This requires some trial-and-error until a more systematic approach is worked out. In fact, some texture and crystal symmetry combinations do not have solutions to produce $\mathcal{A}^{(1)}$ aggregates with isotropic elasticity tensor. (For example, $\mathcal{G}_{\rm cr} = D_6$ with $\mathcal{G}^{(1)} = C_2$ has no solution for $c^2_{00}(R_0) = 0$, $c^2_{02}(R_0) = 0$.) Finally, even if our method successfully produces a solution for a given $\mathcal{G}_{\rm cr}$ and a given set of material tensors $\mathbb{H}^{(i)}$ $(i = 1, ..., s)$, the solution found need not be a minimal solution, i.e., there might still be other arrangements involving a smaller number of $\mathcal{G}_{\rm cr}$-grains for which all the $\mathbb{H}^{(i)}$ tensors of the aggregate are isotropic.

Our ODF method seeks solutions which exhibit texture symmetry. Carrying texture symmetry is clearly not a necessary condition for a solution. A more basic question, which remains to be answered, is whether the set of minimal solutions for a particular $\mathcal{G}_{\rm cr}$ and set of material tensors $\mathbb{H}^{(i)}$, if non-empty, would always include some member that exhibits texture symmetry.

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