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On the Generation of Discrete Isotropic Orientation Distributions for Linear Elastic Cubic Crystals

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Abstract. We consider a model for the elastic behavior of a polycrystalline material based on volume averages. In this case the effective elastic properties depend only on the distribution of the grain orientations. The aggregate is assumed to consist of a finite number of grains each of which behaves elastically like a cubic single crystal. The material parameters are fixed over the grains. An important problem is to find discrete orientation distributions (DODs) which are isotropic, i.e., whose Voigt and Reuss averages of the grain stiffness tensors are isotropic. We succeed in finding isotropic DODs for any even number of grains $N \geqslant 4$ and uniform volume fractions of the grains. Also, $N = 4$ is shown to be the minimum number of grains for an isotropic DOD.

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1. Introduction

During the past decade, simulation techniques for texture evolution and deformation induced anisotropy in polycrystalline materials have been rapidly developed (see Kocks *et al.* [10]). These simulation processes allow the determination of anisotropic mechanical properties of textured polycrystalline materials like metals, minerals, and rocks. In most cases the crystallographic texture, i.e., the inhomogeneity of the distribution of crystal orientations, is of prime importance for the anisotropy of the effective elastic, thermal, or plastic properties.

For the numerical simulations, different approaches like full- and relaxed-constrained Taylor models, self-consistent estimates, and finite element calculations have been applied [10]. All of them have in common that a representative aggregate of the initial material is submitted to an overall deformation or stress process, and its final state is computed by means of micro models from crystal plasticity within the grains. In this context, one of the key problems is the determination of appropriate initial orientations of the grains, which show some prescribed symmetry on the macroscopic level like isotropy. We will call any finite set of orientations

together with their volume fractions a *discrete orientation distribution* (DOD). We are interested in DODs which fulfill two requirements.

- The macroscopic symmetry of the aggregate should meet the prescribed one, either exactly or approximately within a prescribed tolerance.
- The number of orientations needed for that purpose should remain in a range that is practically manageable, in order to avoid an unrealistic computational effort. Often one is interested in DODs with the smallest number of orientations.

Determining DODs by measuring the grain orientations in a region of the real material leads to such large numbers that they clash with the second requirement in most cases. The same problem may be expected when generating DODs as random distributions. There is thus a great need (i) to define precisely the required properties of the DODs in a quantitative way, and (ii) to develop techniques for the generation of DODs that fulfill these requirements.

As a first step to solve this problem, we restrict our concern to the (linear) elastic properties of polycrystalline aggregates, leaving their inelastic properties (flow limit, flow rule, hardening behavior) beyond our considerations. This restriction, which at first glance seems to be rather strong, has been chosen for three reasons.

1. Linear elasticity is a clear and well established mathematical theory, which is not the case for the indefinite area of plasticity or viscoplasticity.
2. The elastic properties within the elastic range of an elastic-plastic material already give us a first insight into the general properties of such aggregates [12].
3. The elastic properties are comparatively easy to determine, both by measurement and calculation and are of considerable practical importance (spring-back analysis in metal forming, wave propagation in geological materials).

It is well-known [9] that the Voigt [14] and Reuss [13] averages give upper and lower bounds for the elastic strain energy of such aggregates independently of the particular grain shape, grain arrangement, and other local features that also influence the effective properties. The bounds were originally developed only for homogeneous orientation distributions, but they were extended to apply to the case of nonhomogeneous distributions [6]. While the bounds can differ significantly from experimental values, the material symmetry is predicted sufficiently well [1]. We will therefore tackle the general problem via the Voigt and Reuss averages.

We note that in the present paper we concentrate on the *cubic* crystal symmetry class. However, the authors presently work on an extended approach, applicable to other symmetry classes. In the subsequent paper Bertram *et al.* [4] we will give isotropic DODs, for any prefixed crystal symmetry class, which involve not more than 12 individual grains.

2. Linear Elastic Behavior

Linear elastic laws can generally be brought into the forms

$$\boldsymbol{T} = \mathbf{C}[\boldsymbol{E}], \quad \text{or, equivalently,} \quad \boldsymbol{E} = \mathbf{S}[\boldsymbol{T}], \tag{2.1}$$

connecting the stress tensor $\boldsymbol{T} \in \mathrm{Sym}(3)$ and the strain tensor $\boldsymbol{E} \in \mathrm{Sym}(3)$. By $\mathrm{Sym}(3)$ we denote the linear space of all real, symmetric (3×3)-matrices (symmetric 2nd-order tensors), endowed with the scalar product $\langle \boldsymbol{A}, \boldsymbol{B}\rangle = \mathrm{trace}(\boldsymbol{AB})$ and the norm $\| \boldsymbol{A} \| = \langle \boldsymbol{A}, \boldsymbol{A}\rangle^{1/2}$, for $\boldsymbol{A}, \boldsymbol{B} \in \mathrm{Sym}(3)$. The (4th-order) stiffness tensor $\mathbf{C}$ and hence also the compliance tensor $\mathbf{S} := \mathbf{C}^{-1}$ are assumed to be self-adjoint and positive-definite linear operators on $\mathrm{Sym}(3)$.

Generally, any linear operator $\mathbf{L} : \mathrm{Sym}(3) \to \mathrm{Sym}(3)$ may be viewed as an element of $\mathbb{R}^{6\times 6}$ (the space of all real (6×6)-matrices), via $\mathbf{L} \cong (\mathrm{L}_{ij})_{1\leqslant i,j\leqslant 6}$ with the definition

$$\mathbf{L}[\boldsymbol{E}_j] = \sum_{i=1}^{6} \mathrm{L}_{ij}\boldsymbol{E}_i, \quad \text{for all } 1 \leqslant j \leqslant 6,$$

referring to a fixed basis $\boldsymbol{E}_1, \ldots, \boldsymbol{E}_6$ of $\mathrm{Sym}(3)$. Throughout, we will work with the particular orthonormal basis of $\mathrm{Sym}(3)$ given by

$$\begin{aligned}
&\boldsymbol{E}_1 = \boldsymbol{e}_1\boldsymbol{e}_1', \qquad \boldsymbol{E}_2 = \boldsymbol{e}_2\boldsymbol{e}_2', \qquad \boldsymbol{E}_3 = \boldsymbol{e}_3\boldsymbol{e}_3',\\
&\boldsymbol{E}_4 = \tfrac{1}{\sqrt{2}}\big(\boldsymbol{e}_1\boldsymbol{e}_3' + \boldsymbol{e}_3\boldsymbol{e}_1'\big), \qquad \boldsymbol{E}_5 = \tfrac{1}{\sqrt{2}}\big(\boldsymbol{e}_2\boldsymbol{e}_3' + \boldsymbol{e}_3\boldsymbol{e}_2'\big),\\
&\boldsymbol{E}_6 = \tfrac{1}{\sqrt{2}}\big(\boldsymbol{e}_1\boldsymbol{e}_2' + \boldsymbol{e}_2\boldsymbol{e}_1'\big),
\end{aligned}$$

where $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$ are the orthonormal unit (column) vectors defining the fixed global coordinate system of $\mathbb{R}^3$, and the prime denotes transposition. Hence we here have

$$\mathrm{L}_{ij} = \langle \boldsymbol{E}_i, \mathbf{L}[\boldsymbol{E}_j]\rangle, \quad \text{for all } 1 \leqslant i, j \leqslant 6.$$

The adjoint linear operator $\mathbf{L}'$ of $\mathbf{L}$ is defined by the condition

$$\langle \boldsymbol{E}, \mathbf{L}[\boldsymbol{F}]\rangle = \langle \mathbf{L}'[\boldsymbol{E}], \boldsymbol{F}\rangle \quad \text{for all } \boldsymbol{E}, \boldsymbol{F} \in \mathrm{Sym}(3),$$

and hence $\mathbf{L}' \cong (\mathrm{L}_{ji})_{1\leqslant i,j\leqslant 6}$ is the transpose of $(\mathrm{L}_{ij})_{1\leqslant i,j\leqslant 6}$. The linear operator $\mathbf{L}$ is called self-adjoint (or Hermitian) if $\mathbf{L}' = \mathbf{L}$, i.e., if its associated matrix is symmetric.

Since the stiffness tensor $\mathbf{C}$ and the compliance tensor $\mathbf{S}$ are self-adjoint and positive-definite linear operators on $\mathrm{Sym}(3)$, they possess spectral decompositions

$$\mathbf{C} = \sum_{i=1}^{\ell} \lambda_i \mathbf{P}_i \quad \text{and} \quad \mathbf{S} = \sum_{i=1}^{\ell} \frac{1}{\lambda_i}\mathbf{P}_i, \tag{2.2}$$

where $\ell \in \{1, \ldots, 6\}$, $\lambda_i > 0$ are the eigenvalues of $\mathbf{C}$, and $\mathbf{P}_i$ are orthogonal projection operators on $\mathrm{Sym}(3)$ projecting onto the corresponding eigenspaces.

The symmetry group $\mathcal{S}$ of the elastic law (2.1) (i.e., the symmetry group of the stiffness tensor $\mathbf{C}$), is the set of all nonsingular real (3×3)-matrices $\boldsymbol{Q}$ such that

$$\mathbf{C}[\boldsymbol{E}] = \boldsymbol{Q}\mathbf{C}[\boldsymbol{Q}'\boldsymbol{E}\boldsymbol{Q}]\boldsymbol{Q}' \quad \text{for all } \boldsymbol{E} \in \mathrm{Sym}(3); \tag{2.3a}$$

actually, as it is easily seen, the *set* of these matrices $\boldsymbol{Q} \in \mathbb{R}^{3\times 3}$ is a *group* (w.r.t. matrix multiplication). We emphasize that in our terminology, $\mathcal{S}$ is the *largest* group of matrices $\boldsymbol{Q}$ satisfying (2.3a), for all $\boldsymbol{E} \in \mathrm{Sym}(3)$.

Upon introducing the linear operator on Sym(3),

$$\mathbf{U}_{\boldsymbol{Q}}[\boldsymbol{E}] = \boldsymbol{Q}\boldsymbol{E}\boldsymbol{Q}' \quad (\boldsymbol{E} \in \mathrm{Sym}(3)), \tag{2.3b}$$

where $\boldsymbol{Q} \in \mathbb{R}^{3\times 3}$, condition (2.3a) can be stated equivalently as an operator identity

$$\mathbf{C} = \mathbf{U}_{\boldsymbol{Q}}\mathbf{C}\mathbf{U}'_{\boldsymbol{Q}}, \tag{2.3c}$$

where the right-hand side of (2.3c) employs the composition of linear operators, and $\mathbf{U}'_{\boldsymbol{Q}}$ stands for the adjoint of $\mathbf{U}_{\boldsymbol{Q}}$. As it is easily seen we have $\mathbf{U}'_{\boldsymbol{Q}} = \mathbf{U}_{\boldsymbol{Q}'}$. Note that (2.3c) may also be viewed as a matrix identity, when identifying linear operators on Sym(3) with the associated (6×6)-matrices.

For solids, any $\boldsymbol{Q} \in \mathcal{S}$ is an orthogonal matrix, and, without loss of generality, we take only those transformations into account which are proper orthogonal, i.e., with $\det \boldsymbol{Q} = +1$. Hence, the symmetry group $\mathcal{S}$ of $\mathbf{C}$ is a subgroup of the special orthogonal group SO(3). If $\mathcal{S}$ coincides with SO(3), the tensor $\mathbf{C}$ is called isotropic. In all other (anisotropic) cases, $\mathcal{S}$ is a proper subgroup of SO(3). An important class of anisotropy is obtained for a cubic single crystal, whose symmetry group is generated by $\pi/2$-rotations around the orthonormal crystal axes vectors $\boldsymbol{g}_i \in \mathbb{R}^3$, $i = 1, 2, 3$. We denote this group by $\mathcal{C}_{\boldsymbol{G}}$, where $\boldsymbol{G}$ stands for the proper orthogonal matrix having $\boldsymbol{g}_1, \boldsymbol{g}_2, \boldsymbol{g}_3$ as columns. $\mathcal{C}_{\boldsymbol{G}}$ contains 24 elements; it is a conjugate group of $\mathcal{C} = \mathcal{C}_{\boldsymbol{I}}$ ($\boldsymbol{I}$ denotes the (3×3)-identity matrix), since $\mathcal{C}_{\boldsymbol{G}} = \boldsymbol{G}\,\mathcal{C}\,\boldsymbol{G}'$, as it is easily seen. In what follows, the cubic crystal class will serve as our standard example on the grain level.

In the isotropic and in the cubic case, the tensor $\mathbf{C}$ has only two and three distinct eigenvalues, resp., and the eigentensors do not depend on the material parameters. Actually, for an isotropic tensor ($\mathcal{S} = \mathrm{SO}(3)$), we have $\ell = 2$ in (2.2) and

$$\begin{aligned} &\mathbf{P}_1 = \tfrac{1}{3}\boldsymbol{I} \otimes \boldsymbol{I}, \quad \text{i.e.,} \quad \mathbf{P}_1[\boldsymbol{E}] = \tfrac{1}{3}\mathrm{trace}(\boldsymbol{E})\boldsymbol{I} \quad \text{for all } \boldsymbol{E} \in \mathrm{Sym}(3), \\ &\mathbf{P}_2 = \mathbf{I}^S - \mathbf{P}_1, \end{aligned} \tag{2.4}$$

where $\boldsymbol{I}$ and $\mathbf{I}^S$ denote the identity matrix in Sym(3) and the identity operator on Sym(3), respectively. In the cubic case ($\mathcal{S} = \mathcal{C}_{\boldsymbol{G}}$), we have $\ell = 3$ and the three orthogonal projection operators (projecting onto the eigenspaces of $\mathbf{C} = \mathbf{C}_{\boldsymbol{G}}$)

$$\mathbf{P}_1 = \tfrac{1}{3}\boldsymbol{I} \otimes \boldsymbol{I}, \qquad \mathbf{P}_{2,\boldsymbol{G}} = \mathbf{D}_{\boldsymbol{G}} - \mathbf{P}_1, \qquad \mathbf{P}_{3,\boldsymbol{G}} = \mathbf{I}^S - \mathbf{D}_{\boldsymbol{G}}, \tag{2.5}$$

where $\boldsymbol{G}$ has the orthonormal crystal lattice vectors $\boldsymbol{g}_i$ as columns, and

$$\mathbf{D}_{\boldsymbol{G}} = \sum_{i=1}^{3} (\boldsymbol{g}_i\,\boldsymbol{g}_i') \otimes (\boldsymbol{g}_i\,\boldsymbol{g}_i'), \tag{2.6}$$

that is, $\mathbf{D}_G[E] = \sum_{i=1}^{3}(g_i' E g_i)g_i g_i'$ for all $E \in \mathrm{Sym}(3)$; cf. Bertram and Olschewski [2, 3]. Note that $\mathbf{D}_G$ is the orthogonal projection operator on Sym(3) projecting onto the linear subspace spanned by $g_i g_i'$, $i = 1, 2, 3$.

3. Averages of Elastic Laws and Isotropy

The standard problem of homogenization for polycrystalline materials can be described as follows. We consider an aggregate of N grains forming a representative volume element. The difference of the material between different grains lies only in the fact that they are differently oriented in space. A *discrete orientation distribution* (DOD) is given by a set of N pairs (G_j, ξ_j), $j = 1, \ldots, N$, where $G_j \in \mathrm{SO}(3)$ describes the orientation and $\xi_j > 0$ the volume fraction of the grain. Note that $\sum_{j=1}^{N} \xi_j = 1$. The number N of grains will be called the *size* of the DOD. Henceforth, each grain is supposed to behave like a cubic single crystal, i.e., the symmetry group of a grain with orientation G is the group $\mathcal{C}_G$ from above. Thus, according to (2.2) and (2.5), the elastic behavior of $\mathbf{C}_G$ is given by its stiffness and compliance tensors,

$$\begin{aligned} \mathbf{C}_G &= \lambda_1 \mathbf{P}_1 + \lambda_2 \mathbf{P}_{2,G} + \lambda_3 \mathbf{P}_{3,G}, \\ \mathbf{S}_G &= \frac{1}{\lambda_1}\mathbf{P}_1 + \frac{1}{\lambda_2}\mathbf{P}_{2,G} + \frac{1}{\lambda_3}\mathbf{P}_{3,G}, \end{aligned} \tag{3.1}$$

where the positive eigenvalues $\lambda_1, \lambda_2, \lambda_3$ are fixed (the same for all grains). Since the symmetry group of $\mathbf{C}_G$ is assumed to be precisely the cubic group $\mathcal{C}_G$, we implicitly have $\lambda_2 \neq \lambda_3$: For, otherwise, $\mathbf{C}_G = \lambda_1 \mathbf{P}_1 + \lambda_2 \mathbf{P}_2$ (with $\mathbf{P}_2$ from (2.4)), is itself isotropic, and SO(3) is the associated symmetry group, for all G.

The problem is to determine the (macroscopic) behavior of the aggregate given by a DOD, i.e., the effective stiffness tensor $\mathbf{C}^A$ or the effective compliance tensor $\mathbf{S}^A = (\mathbf{C}^A)^{-1}$. We will employ the Voigt and the Reuss averages, $\mathbf{C}^V$ and $\mathbf{C}^R$, resp., given by

$$\mathbf{C}^V = \sum_{j=1}^{N} \xi_j \mathbf{C}_{G_j} \quad \text{and} \quad \mathbf{C}^R = (\mathbf{S}^R)^{-1}, \quad \text{where } \mathbf{S}^R = \sum_{j=1}^{N} \xi_j \mathbf{S}_{G_j}.$$

It is well-known that the Voigt average describes the aggregate under the assumption of homogeneous strains, and the Reuss average under homogeneous stresses. These cases define the two extremes of the strain energy density, since

$$\begin{aligned} &\mathbf{C}^R \leqslant \mathbf{C}^A \leqslant \mathbf{C}^V, \quad \text{i.e.,} \\ &\langle E, \mathbf{C}^R[E]\rangle \leqslant \langle E, \mathbf{C}^A[E]\rangle \leqslant \langle E, \mathbf{C}^V[E]\rangle \quad \text{for all } E \in \mathrm{Sym}(3). \end{aligned}$$

This is one important property of these two averages. Another one lies in the fact that they both are independent of the form and location of the grains, but depend only on the crystal data and the DOD. In contrast to this, the aggregate stiffness $\mathbf{C}^A$

showing validity of (4.8).

(3) We show existence of an isotropic, *elementary* $\mathcal{Q}$-symmetric DOD.

To this end, we first note that, by Lemma 4.1, there exists an isotropic, $\mathcal{Q}$-symmetric DOD,

$$\big(\boldsymbol{Q}_i \boldsymbol{G}_k, w_k/r\big), \quad 1 \leqslant i \leqslant r,\ 1 \leqslant k \leqslant s,$$

for some $s \in \mathbb{N}$, $\boldsymbol{G}_1, \ldots, \boldsymbol{G}_s \in \mathrm{SO}(3)$, and $w_1, \ldots, w_s > 0$ with $\sum_{k=1}^{s} w_k = 1$. By Lemma 3.1 and (4.3),

$$\sum_{k=1}^{s} w_k \overline{\mathbf{D}}^{\mathcal{Q}}_{\boldsymbol{G}_k} = \mathbf{P}_1 + \tfrac{2}{5}\mathbf{P}_2. \tag{4.9}$$

The left-hand side of (4.9) is an element of the convex hull of the set

$$\big\{\overline{\mathbf{D}}^{\mathcal{Q}}_{\boldsymbol{G}} : \boldsymbol{G} \in \mathrm{SO}(3)\big\}. \tag{4.10}$$

By (4.7a) and (4.7b), the set (4.10) is already convex, since $f(\boldsymbol{G})$ is a continuous real valued function of $\boldsymbol{G} \in \mathrm{SO}(3)$, the group SO(3) is connected (cf. Curtis [7], page 89 and Chapter VIII), and thus the values $f(\boldsymbol{G})$, when $\boldsymbol{G}$ ranges over SO(3), constitute a compact interval of the real line. We conclude that there is a $\boldsymbol{G} \in \mathrm{SO}(3)$ such that $\sum_{k=1}^{s} w_k \overline{\mathbf{D}}^{\mathcal{Q}}_{\boldsymbol{G}_k} = \overline{\mathbf{D}}^{\mathcal{Q}}_{\boldsymbol{G}}$. By (4.9), Lemma 3.1, and (4.1a), the associated elementary $\mathcal{Q}$-symmetric DOD $(\boldsymbol{Q}_i \boldsymbol{G}, 1/r)$, $1 \leqslant i \leqslant r$, is isotropic.

(4) Consider an arbitrary elementary $\mathcal{Q}$-symmetric DOD $(\boldsymbol{Q}_i \boldsymbol{G}, 1/r)$, $1 \leqslant i \leqslant r$, where $\boldsymbol{G} \in \mathrm{SO}(3)$. By Lemma 3.1, the DOD is isotropic if and only if $\overline{\mathbf{D}}^{\mathcal{Q}}_{\boldsymbol{G}} = \mathbf{P}_1 + \frac{2}{5}\mathbf{P}_2$. By (4.7a), (2.5), and (2.4), the latter identity is equivalent to $\frac{1}{2}(f(\boldsymbol{G}) - 1) = 1 - \frac{1}{3}f(\boldsymbol{G}) = 2/5$, i.e., to $f(\boldsymbol{G}) = 9/5$. Now (4.8) completes the proof. □

5. Construction of Isotropic DODs

We will find isotropic, elementary $\mathcal{C}^*$-symmetric DODs, where $\mathcal{C}^*$ is the subgroup from (4.5). These isotropic DODs will be of size 12. Some of them will be further reduced to isotropic DODs of smaller sizes, in particular, to the minimum size of four (see below).

By Theorem 4.2, an isotropic, elementary $\mathcal{C}^*$-symmetric DOD is given by a solution to the equation

$$f(\boldsymbol{G}) = \tfrac{9}{5}, \tag{5.1}$$

where $f(\boldsymbol{G}) = \sum_{i=1}^{3}\sum_{j=1}^{3} g_{ij}^4$, $\boldsymbol{G} = (g_{ij})_{1 \leqslant i,j \leqslant 3}$.

The following representation of SO(3) will be useful for deriving solutions to (5.1). By Curtis [7], pages 60 ff., the group SO(3) is the image under a group

homomorphism of the unit sphere in $\mathbb{R}^4$ (considered as a multiplicative subgroup of the noncommutative field of quaternions). Explicitly, this reads as

$$\boldsymbol{G}(\boldsymbol{x}) = \begin{pmatrix} x_1^2 + x_2^2 - x_3^2 - x_4^2 & -2x_1x_4 + 2x_2x_3 & 2x_1x_3 + 2x_2x_4 \\ 2x_1x_4 + 2x_2x_3 & x_1^2 - x_2^2 + x_3^2 - x_4^2 & -2x_1x_2 + 2x_3x_4 \\ -2x_1x_3 + 2x_2x_4 & 2x_1x_2 + 2x_3x_4 & x_1^2 - x_2^2 - x_3^2 + x_4^2 \end{pmatrix},$$

$$\boldsymbol{x} = (x_1, x_2, x_3, x_4) \in \mathbb{R}^4, \quad \sum_{i=1}^{4} x_i^2 = 1.$$

By some lengthy, but elementary calculations we find

$$\begin{aligned} f\big(\boldsymbol{G}(\boldsymbol{x})\big) \;=\; & \big(x_1^2 + x_2^2 - x_3^2 - x_4^2\big)^4 + \big(x_1^2 - x_2^2 + x_3^2 - x_4^2\big)^4 \\ & + \big(x_1^2 - x_2^2 - x_3^2 + x_4^2\big)^4 + 32\Big(\big(x_1^2x_4^2 + x_2^2x_3^2\big)^2 \\ & + \big(x_1^2x_3^2 + x_2^2x_4^2\big)^2 + \big(x_1^2x_2^2 + x_3^2x_4^2\big)^2\Big) + 384x_1^2x_2^2x_3^2x_4^2. \end{aligned}$$

Substituting $z_i = x_i^2$, $i = 1, 2, 3, 4$, we see that this expression becomes a polynomial $p(z)$, say, of fourth degree in the four-dimensional variable $z = (z_1, z_2, z_3, z_4)$, and (5.1) becomes

$$p(z) = 9/5, \quad z_i \geqslant 0 \text{ for all } i = 1, \ldots, 4, \text{ and } \sum_{i=1}^{4} z_i = 1. \tag{5.2}$$

Consider two particular line segments in the simplex of z vectors,

$$z(\lambda) = \big(0, \lambda, (1-\lambda)/2, (1-\lambda)/2\big) \quad \text{for } \lambda \in [0, 1], \tag{5.3a}$$

and

$$z(\rho) = \big(\rho, (1-\rho)/3, (1-\rho)/3, (1-\rho)/3\big) \quad \text{for } \rho \in [0, 1], \tag{5.3b}$$

both of which contain points which solve (5.2). Choosing $\lambda = 0$ and $\lambda = 1/3$ in (5.3a), we get $p(0, 0, 1/2, 1/2) = 3 > 9/5 > 11/9 = p(0, 1/3, 1/3, 1/3)$; choosing in (5.3b) $\rho = 0$ and $\rho = 1$, we find $p(0, 1/3, 1/3, 1/3) = 11/9 < 9/5 < 3 = p(1, 0, 0, 0)$.

For (5.3a), an elementary calculation shows

$$p\big(z(\lambda)\big) = 36\big(\lambda(1-\lambda)\big)^2 - 16\lambda(1-\lambda) + 3,$$

and (5.2) becomes $\lambda(1-\lambda) = \frac{2}{9} - \sqrt{\frac{4}{81} - \frac{1}{30}}$, leading to

$$\lambda = \frac{1}{2} \pm \sqrt{\frac{1}{36} + \sqrt{\frac{4}{81} - \frac{1}{30}}}$$

and

$$\boldsymbol{x} = \left(0, \pm\sqrt{\lambda}, \pm\sqrt{\frac{1}{2}(1-\lambda)}, \pm\sqrt{\frac{1}{2}(1-\lambda)}\right).$$

For example, taking

$$\lambda = \frac{1}{2} + \sqrt{\frac{1}{36} + \sqrt{\frac{4}{81} - \frac{1}{30}}} \quad \text{and} \quad \boldsymbol{x} = \left(0, \sqrt{\lambda}, \sqrt{\frac{1}{2}(1-\lambda)}, \sqrt{\frac{1}{2}(1-\lambda)}\right)$$

we obtain as a solution $\boldsymbol{G} = \boldsymbol{G}(\boldsymbol{x})$ to (5.1) (defining thus an isotropic DOD of size 12 with uniform volume fractions 1/12),

$$\boldsymbol{G} = \begin{pmatrix} 0.78604 & 0.43712 & 0.43712 \\ 0.43712 & -0.89302 & 0.10698 \\ 0.43712 & 0.10698 & -0.89302 \end{pmatrix}. \tag{5.4}$$

For (5.3b), we find by an elementary calculation that

$$9p\big(z(\rho)\big) = 256\rho^3 - 384\rho^2 + 144\rho + 11, \tag{5.5}$$

and the cubic equation $p\big(z(\rho)\big) = 9/5$ is found to have the three solutions

$$\rho_i = \frac{1}{2}\left(1 - \cos\left(\frac{\varphi + 2i\pi}{3}\right)\right), \quad i = 1, 2, 3, \text{ where } \cos(\varphi) = 7/20. \tag{5.6}$$

For any of these ρ-values, and with

$$\boldsymbol{x} = \left(\sqrt{\rho}, \pm\sqrt{(1-\rho)/3}, \pm\sqrt{(1-\rho)/3}, \pm\sqrt{(1-\rho)/3}\right),$$

solutions $\boldsymbol{G} = \boldsymbol{G}(\boldsymbol{x})$ to (5.1) are then identifiable (thus defining isotropic DODs of size 12 with uniform volume fractions 1/12). For example, for

$$\boldsymbol{x} = (\sqrt{\rho_1}, \sqrt{(1-\rho_1)/3}, \sqrt{(1-\rho_1)/3}, \sqrt{(1-\rho_1)/3})$$

we get

$$\boldsymbol{G} = \begin{pmatrix} -0.27956 & 0.41261 & 0.86695 \\ 0.86695 & -0.27956 & 0.41261 \\ 0.41261 & 0.86695 & -0.27956 \end{pmatrix}. \tag{5.7}$$

As a third easy approach for getting special solutions to (5.1) we consider matrices of the type

$$\boldsymbol{G} = \begin{pmatrix} 0 & 1/\sqrt{2} & 1/\sqrt{2} \\ \beta & -\sqrt{(1-\beta^2)/2} & \sqrt{(1-\beta^2)/2} \\ \sqrt{1-\beta^2} & \beta/\sqrt{2} & -\beta/\sqrt{2} \end{pmatrix},$$
$$\text{for } \beta \in [-1, 1]. \tag{5.8a}$$

By an easy calculation one finds that such a matrix satisfies (5.1) if and only if

$$\beta^4 - \beta^2 + \frac{1}{15} = 0, \quad \text{that is,} \quad \beta = \pm\sqrt{\frac{1}{2} \pm \sqrt{\frac{1}{4} - \frac{1}{15}}}, \tag{5.8b}$$

thus defining further isotropic DODs of size 12 with uniform volume fractions $1/12$.

It may happen that an elementary $\mathcal{C}^*$-symmetric isotropic DOD, like the above, actually constitutes an isotropic DOD of even smaller size. This is due to the invariance property of the stiffness tensor $\mathbf{C}_G$, for any given $\boldsymbol{G} \in \mathrm{SO}(3)$,

$$\mathbf{C}_{GR} = \mathbf{C}_G \quad \text{for all } \boldsymbol{R} \in \mathcal{C}, \tag{5.9a}$$

and similarly,

$$\mathbf{D}_{GR} = \mathbf{D}_G \quad \text{for all } \boldsymbol{R} \in \mathcal{C}; \tag{5.9b}$$

here, $\mathcal{C}$ is the full cubic group introduced in Section 2. Equations (5.9a) and (5.9b) can be verified as follows. The conjugate group $\mathcal{C}_G = \boldsymbol{G}\mathcal{C}\boldsymbol{G}'$ has been identified as a symmetry group of $\mathbf{C}_G$ (see Section 2), i.e.,

$$\mathbf{C}_G = \mathbf{U}_{GRG'}\mathbf{C}_G\mathbf{U}'_{GRG'} \quad \text{for all } \boldsymbol{R} \in \mathcal{C}. \tag{5.10}$$

By (3.4a), (3.1), (2.5), and by the isotropy of $\mathbf{P}_1$ and $\mathbf{I}^S$, we have

$$\mathbf{C}_{QG} = \mathbf{U}_Q\mathbf{C}_G\mathbf{U}'_Q \quad \text{for all } \boldsymbol{Q} \in \mathrm{SO}(3).$$

From this and (5.10) we obtain (5.9a) when specializing to $\boldsymbol{Q} = \boldsymbol{GRG}'$ with any $\boldsymbol{R} \in \mathcal{C}$. Equation (5.9b) is an immediate consequence from (5.9a) and (3.1), (2.5).

In view of (5.9a), (5.9b) the relation on SO(3),

$$\boldsymbol{H} \sim \boldsymbol{K} \iff \text{there exists an } \boldsymbol{R} \in \mathcal{C} \text{ such that } \boldsymbol{H} = \boldsymbol{KR} \tag{5.11}$$

(for $\boldsymbol{H}, \boldsymbol{K} \in \mathrm{SO}(3)$), will be meaningful. As it is well known (and easily seen), (5.11) is an equivalence relation on SO(3), the equivalence classes of which are the sets $\boldsymbol{G}\mathcal{C}$, where $\boldsymbol{G} \in \mathrm{SO}(3)$. As a consequence for an isotropic DOD, orientations included in the DOD which belong to the same equivalence class can be replaced by one single representative of that equivalence class without affecting isotropy, thus leading to an isotropic DOD of possibly smaller size. Inspecting this for the isotropic elementary $\mathcal{C}^*$-symmetric DODs of size 12 given by (5.4), (5.7), and (5.8a), (5.8b), we obtain no reduction for (5.4), but we do obtain a reduction for the other solutions: A DOD given by (5.7) reduces to a DOD of size four with uniform volume fractions $1/4$ the orientations of which can be chosen as

$$\boldsymbol{G}, \boldsymbol{D}_1\boldsymbol{G}, \boldsymbol{D}_2\boldsymbol{G}, \boldsymbol{D}_3\boldsymbol{G}, \tag{5.12}$$

with $\boldsymbol{G}$ from (5.7) (where $\boldsymbol{D}_i$, $i = 1, 2, 3$, have been defined in (4.5)). A DOD given by (5.8a), (5.8b), reduces to a DOD of size six with uniform volume fractions $1/6$ the orientations of which can be chosen as

$$\boldsymbol{G}, \boldsymbol{D}_2\boldsymbol{G}, \boldsymbol{D}_3\boldsymbol{G}, \boldsymbol{AG}, \boldsymbol{A}^2\boldsymbol{G}, \boldsymbol{D}_1\boldsymbol{AG},$$

with $\boldsymbol{G}$ from (5.8a), (5.8b) (and $\boldsymbol{A}$ from (4.5)).

In particular, since we have thus constructed isotropic DODs of size four and size six with uniform volume fractions, we can obtain isotropic DODs with uniform volume fractions of any even size $N \geqslant 4$, by simply combining appropriate numbers of isotropic DODs of sizes four and six.

An isotropic DOD of size eight and with uniform volume fractions 1/8 has been constructed by Krawietz [11]. However, we note that his solution consists of two isotropic DODs each of size four as given by (5.12), though equivalently transformed according to the equivalence relation (5.11). More precisely, the orientations employed in [11] are given by

$$\boldsymbol{G}(\boldsymbol{x}_i),\ \boldsymbol{D}_1\boldsymbol{G}(\boldsymbol{x}_i)\boldsymbol{D}_1,\ \boldsymbol{D}_2\boldsymbol{G}(\boldsymbol{x}_i)\boldsymbol{D}_2,\ \boldsymbol{D}_3\boldsymbol{G}(\boldsymbol{x}_i)\boldsymbol{D}_3, \quad i = 1, 2,$$

with $\boldsymbol{x}_{1;2} = (\sqrt{\rho}, \pm\sqrt{(1-\rho)/3}, \pm\sqrt{(1-\rho)/3}, \pm\sqrt{(1-\rho)/3})$ and $\rho \in \{\rho_1, \rho_2, \rho_3\}$ from (5.6).

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