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Material Tensors and Pseudotensors of Weakly-Textured Polycrystals with Orientation Measure Defined on the Orthogonal Group

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MATERIAL TENSORS AND PSEUDOTENSORS OF WEAKLY-TEXTURED POLYCRYSTALS WITH ORIENTATION MEASURE DEFINED ON THE ORTHOGONAL GROUP

DISSERTATION

A dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in the College of Arts and Sciences at the University of Kentucky

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ABSTRACT OF DISSERTATION

MATERIAL TENSORS AND PSEUDOTENSORS OF WEAKLY-TEXTURED POLYCRYSTALS WITH ORIENTATION MEASURE DEFINED ON THE ORTHOGONAL GROUP

Material properties of polycrystalline aggregates should manifest the influence of crystallographic texture as defined by the orientation distribution function (ODF). A representation theorem on material tensors of weakly-textured polycrystals was established by Man and Huang (2012), by which a given material tensor can be expressed as a linear combination of an orthonormal set of irreducible basis tensors, with the components given explicitly in terms of texture coefficients and a number of undetermined material parameters. Man and Huang's theorem is based on the classical assumption in texture analysis that ODFs are defined on the rotation group SO(3), which strictly speaking makes it applicable only to polycrystals with (single) crystal symmetry defined by a proper point group. In the present study we consider ODFs defined on the orthogonal group O(3) and extend the representation theorem of Man and Huang to cover pseudotensors and polycrystals with crystal symmetry defined by any improper point group. This extension is important because many materials, including common metals such as aluminum, copper, iron, have their group of crystal symmetry being an improper point group. We present the restrictions on texture coefficients imposed by crystal symmetry for all the 21 improper point groups, and we illustrate the extended representation theorem by its application to elasticity.

KEYWORDS: Materials tensors and pseudotensors, Polycrystals, Orthogonal group, Texture, Elasticity

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Chapter 1 Introduction

Many materials are polycrystalline aggregates of tiny crystallites or grains of various sizes and shapes separated by defective boundaries. In theories to evaluate physical properties of a polycrystal, as a first approximation, all effects of grain boundaries are ignored and the constituent crystallites of the polycrystal are taken as parts of perfect single crystals, the crystal lattices of which have different orientations in space. Since each crystallite is anisotropic, the macroscopic physical properties of the polycrystal will likewise be anisotropic unless the orientations of its constituent crystallites are completely random. However, manufacturing processes (e.g. annealing and hot/cold rolling in the case of sheet metals) usually impart material products with crystallographic texture, i.e., the constituent crystallites have preferred orientations. In materials science, orientation distribution functions (ODFs) defined on the rotation group (SO(3)) have been used to characterize crystallographic texture (see, e.g., the monograph by Bunge [5]).

Material properties are often described by tensors or pseudotensors of various types. Material tensors and pseudotensors pertaining to polycrystalline aggregates should manifest the influence of crystallographic texture on material properties. Many papers which study the effects of texture on various material properties have been published. But, until the recent work of Man and Huang [20], all these papers were restricted to some specific classes of tensors (e.g. second-order tensors that describe thermal conductivity, optical refractive index and electrical conductivity, the fourth-order elasticity tensor, the sixth-order acoustoelastic tensor, etc.) and, with one exception (namely, Morris' computation [27] of the Voigt average of the fourth-order elasticity tensor for polycrystals with both texture and crystal symmetry described by any rotational point group), were restricted to some specific texture and crystal symmetries (e.g., orthorhombic aggregates of cubic or hexagonal crystallites were mostly studied). Man and Huang [20] derived a representation theorem by which any material tensor of a weakly-textured polycrystal can be expressed as a linear combination of an orthonormal set of irreducible basis tensors, with the components given explicitly in terms of texture coefficients and a set of undetermined material parameters. In their paper they provide a procedure by which the irreducible basis tensors can be constructed explicitly. The representation theorem of Man and Huang is based on the classical assumption in quantitative texture analysis that the ODF is defined on the rotation group. As a consequence, both texture symmetry and crystal symmetry are described by subgroups of the rotation group.

Among the 32 crystallographic point groups, 11 are proper (i.e., they are subgroups of SO(3)) and 21 are improper (i.e., they are subgroups of O(3) but not SO(3)). A survey ([29], Section 3.5) of circa 127,000 inorganic and 156,000 organic compounds shows that only 9.15% of the inorganic and 19.71% of the organic crystals have their symmetries described by rotational point groups; the rest, which is a huge majority by abundance, has their symmetries described by improper point groups. In fact, in texture analysis the importance of relaxing the restriction to crystallites with symmetries described by rotational point groups is indicated not only by the aforementioned population statistics, but also by the fact that many engineering materials (e.g., metals such as aluminum, copper, iron, magnesium, titanium, zinc) have some improper point group as their group of crystal symmetry (G_{cr}).

With the abundance and importance of materials whose crystal symmetry groups are improper, one may wonder why material scientists would develop texture analysis with ODFs defined on SO(3). Here we venture to give two plausible explanations:

(1) Quantitative texture analysis began in the 1960s. At that time X-ray diffraction (XRD) was the only tool that could deliver quantitative information on the ODF. By Friedel's law, XRD can not distinguish two crystals that have their G_{cr} in the same Laue class, each of which has one rotational point group as member. For example,

aluminum crystals have their $G_{\mathrm{cr}} = O_h$, an improper point group. The diffraction pattern would be the same even if the proper point group O, a peer of O_h in the same Laue class, were the symmetry group of aluminum crystals.

(2) The predictions made by the SO(3)-based texture analysis were confirmed by experiments in various fields, e.g., in ultrasonics.

With the advent and development of orientation imaging microscopy in the last two decades, however, we now have tools more powerful than XRD for texture measurement. As for (2), that the SO(3)-based texture analysis works for some problems which involve materials with their G_{cr} being some improper point group is no proof that it will always work for all such problems. In this regard, a few questions naturally arise:

- Will the SO(3)-based texture analysis always work?
- If the answer to the preceding question is negative, why did the SO(3)-based texture analysis work for so many problems? What are the conditions that make it work for those problems?

The main objective of this thesis is to extend the representation theorem of Man and Huang [20] by letting the ODF be defined on the orthogonal group O(3) so that the extended theorem will cover also aggregates of crystallites with their G_{cr} being an improper point group. With the extended theorem in hand, we will answer the questions above at least for material properties of weakly-textured polycrystals that are characterized by tensors or pseudotensors. We will also examine some applications of the extended theorem in elasticity. It should be pointed out that it was Bunge and his coworkers [5, 6, 7, 8] who first examined ODFs defined on O(3). Their attention, however, was largely restricted to the effects of texture and crystal symmetry on the ODF and the possibility of measurement of the O(3)-based ODF by XRD. Here we are mainly interested in the effects of texture on material properties that are characterized by tensors and pseudotensors.

What follows is an outline of the contents of this thesis. In Chapter 2, we recapitulate some basic concepts and facts about crystallographic point groups (i.e., finite subgroups of the orthogonal group O(3) that satisfy the crystallographic restriction), integration on O(3), group representations, and material tensors and pseudotensors. We begin Chapter 3 by presenting a complete set of irreducible representations of O(3). Perhaps because such a complete set for O(3) can be easily obtained from a complete set of irreducible representations of SO(3), this information is seldom presented in books and, in the few instances [1, 24] where this information is touched upon, it is mentioned only in passing. On the other hand, the irreducible representations of O(3) play a central role in the present study. Hence in Sections 3.1 and 3.2 we derive in detail all the information on a complete set of irreducible representations of O(3) that we need. Building on these prerequisites, in Section 3.3 we obtain Theorem 3.3.3, which describes how the rank of a tensor or pseudotensor affects its decomposition into irreducible parts under O(3). Chapter 4 is the centerpiece of this thesis, where we adopt the approach to texture analysis originated by Roe [32, 33]. In Section 4.2 we introduce ODFs defined on O(3) and explain how an aggregate of crystallites with their $G_{\rm cr}$ being an improper point group can be looked upon as a mixture of right-handed and left-handed crystals given in equal volume fractions. It is this observation and the main physical assumption (4.3.1), which is none other than a version of the "principle of material frame-indifference" [39] for our present context, that serve as the basis for the proof of Theorem (4.6.4), the extended representation theorem that we seek. In Section 4.7 we present an alternative line of argument, which appeals heavily to Man and Huang's original representation theorem, to arrive at the extended representation theorem. In Chapter 5, using an argument similar to that given by Roe [32, 33] in SO(3)-based texture analysis, we extend the transformation formula for texture coefficients under change of reference crystal orientation so that the new formulas are valid when the ODF is defined on O(3). We then apply the transformation formulas to derive restrictions on texture coefficients imposed by crystal symmetry for each of the 32 crystallographic point groups. The parallel problem—regarding the effects of crystal symmetry on the O(3)-based ODF—in Bunge's approach [5] to texture analysis was examined in a 1981 paper by Bunge, Esling, and Muller [7]. We close the thesis in Chapter 6 by applying the representation theorem (4.6.4) and the restrictions on texture coefficients derived in Chapter 5 to material tensors and pseudotensors of single crystals in $[[V_c^{\otimes 2}]^{\otimes 2}]$, the space of 4th-order tensors and pseudotensors that enjoy both the major and minor symmetries. There we derive the explicit form of the 6×6 matrices that represent, in the Voigt notation, material tensors and pseudotensors of single crystals with G_{cr} being C_s, D_{3h}, C_{4v}, or D_{2d}, which are Type III improper groups. We present also the number of undetermined material parameters (UMP) for the class of material tensors and pseudotensors that we obtain by our method for single crystals with any of the 10 Type III improper groups as G_{cr}. This exercise serves as a check on the correctness of the representation formula (4.94) and the restrictions derived in Chapters 4 and 5, respectively, because the aforementioned matrices and UMPs can be derived by brute force, i.e., by exploiting the fact that the material tensor and pseudotensor at issue remain invariant under transformations induced by elements of the symmetry group in question (cf. (2.38) and (2.39)). We use Type III crystal and even-order pseudotensor for this check because this represents the situation where the representation formula differs most markedly from its counterpart for the Type I crystal which is its peer in the same Laue class.

Chapter 2 Preliminaries

2.1 Crystallographic point groups

2.1.1 Definition

The orthogonal group of dimension 3, denoted by O(3), is the group of distance and angle preserving transformations of a Euclidean space of dimension 3 that preserve a fixed point, where the group operation is given by composing transformations [18]. Equivalently, it is the group of 3×3 orthogonal matrices. These matrices form a group because they are closed under multiplication and taking inverses. An orthogonal matrix is a real matrix whose inverse equals its transpose. Let $\boldsymbol{E}$ and $\boldsymbol{Q}$ denote the identity and any element in O(3), respectively, then we have $\boldsymbol{Q}\boldsymbol{Q}^T = \boldsymbol{Q}^T\boldsymbol{Q} = \boldsymbol{E}$ [18, 26, 35].

The determinant of an orthogonal matrix is either 1 or -1. A very important subgroup of O(3) is the special orthogonal group, denoted by SO(3), of the orthogonal matrices with determinant 1. This group is also called the rotation group since its elements are the usual rotations around an axis in dimensions 3.

Except for the identity $\boldsymbol{E}$, every rotation $\boldsymbol{R} \in \mathrm{SO}(3)$ is specified [18] by an axis and an angle of rotation. Let $\boldsymbol{R}(\boldsymbol{n}, \omega)$ denote the rotation with the axis defined by the unit vector $\boldsymbol{n}$ and with angle of rotation ω. Extending this notation, we let $\boldsymbol{R}(\boldsymbol{n}, 0) = \boldsymbol{E}$ for any $\boldsymbol{n}$. To cover the entire rotation group, we may limit $\omega \in [0, \pi]$ because $\boldsymbol{R}(-\boldsymbol{n}, \theta) = \boldsymbol{R}(\boldsymbol{n}, 2\pi - \theta)$.

A rotation $\boldsymbol{R}(\boldsymbol{n}, \omega)$ is a symmetry operation of a crystal lattice if it renders the lattice invariant. With this, the lattice structure imposes a severe restriction on the possible values of rotation angle ω of the symmetry operation $\boldsymbol{R}(\boldsymbol{n}, \omega)$ [18, 35]. It can be shown that the trace of $\boldsymbol{R}(\boldsymbol{n}, \omega)$ is $1 + 2\cos\omega$ which should be an integer. Within the range of $[0, \pi]$, the possible values of ω are $0, \frac{\pi}{3}, \frac{\pi}{2}, \frac{2\pi}{3}, \pi$. This requirement on the rotation angle ω is called the crystallogaphic restriction on the symmetry operation $\boldsymbol{R}(\boldsymbol{n}, \omega)$ of a crystal lattice.

Finite subgroups of O(3) are called point groups. Those that further satisfy the crystallographic restriction are called crystallographic point groups.

2.1.2 Classification

Crystallographic point groups that only contain rotational operators are called proper groups, while groups with both rotations and reflections (combination of rotation and inversion denoted as $\boldsymbol{I}$) are called improper groups in many references (e.g. [2, 3, 4, 35, 37]). In what follows we denote generic proper and improper groups by G_p and G_i, respectively.

There are 11 finite subgroups of the rotational group SO(3) that satisfy the crystallogaphic restriction [2, 18, 35]. These 11 subgroups in the Schönflies notation are C_1, C_2, C_3, C_4, C_6, D_2, D_3, D_4, D_6, T, and O, where C_n, D_n, T, and O are referred to as the cyclic, dihedral, tetrahedral, and octahedral (cubic) groups respectively. Clearly these 11 finite subgroups of SO(3) are the proper (rotational) crystallographic point groups since SO(3) is a subgroup of O(3).

The structure of the improper crystallographic point groups can be ascertained through the following theorems [35].

Theorem 2.1.1. [35] *Any improper group can be decomposed into a proper subgroup and its coset, i.e.,* $G_i = G_p \bigcup \bar{\boldsymbol{R}} G_p$*, where* $\bar{\boldsymbol{R}} = \boldsymbol{IR}$ *is an improper operator (inversion-rotation).*

Proof. Clearly all proper operators $\boldsymbol{E} = \boldsymbol{R}_1, \boldsymbol{R}_2, ..., \boldsymbol{R}_j, ..., \boldsymbol{R}_n$ in G_i form a proper subgroup, say G_p. Let $\bar{\boldsymbol{R}}$ be any improper operator in G_i. Then $\bar{\boldsymbol{R}} G_p = \{\bar{\boldsymbol{R}}, \bar{\boldsymbol{R}}\boldsymbol{R}_2, ..., \bar{\boldsymbol{R}}\boldsymbol{R}_j, ..., \bar{\boldsymbol{R}}\boldsymbol{R}_n\}$. To complete the proof, it suffices to show any other improper element $\bar{\boldsymbol{R}}'$ in G_i is in $\bar{\boldsymbol{R}} G_p$. Indeed, since $\bar{\boldsymbol{R}}^2$ and $\bar{\boldsymbol{R}}\bar{\boldsymbol{R}}'$ are proper elements, there exists a j and a k, such that $\bar{\boldsymbol{R}}^2 = \boldsymbol{R}_j$ and $\bar{\boldsymbol{R}}\bar{\boldsymbol{R}}' = \boldsymbol{R}_k$. Thus $\bar{\boldsymbol{R}}' = \bar{\boldsymbol{R}}^{-1}\boldsymbol{R}_k = \bar{\boldsymbol{R}}^{-1}\boldsymbol{R}_j\boldsymbol{R}_j^{-1}\boldsymbol{R}_k = \bar{\boldsymbol{R}}^{-1}\bar{\boldsymbol{R}}\bar{\boldsymbol{R}}\boldsymbol{R}_j^{-1}\boldsymbol{R}_k = \bar{\boldsymbol{R}}\boldsymbol{R}_j^{-1}\boldsymbol{R}_k = \bar{\boldsymbol{R}}\boldsymbol{R}_m$ for some m, which is in $\bar{\boldsymbol{R}} G_p$. □

With this theorem, we have one type of improper crystallographic point groups: Improper groups that contain the inversion as a member can be decomposed as the disjoint union of G_p and its coset $\boldsymbol{I}G_p$, i.e., $G_i = G_p \bigcup \boldsymbol{I}G_p$. These 11 improper groups in the Schönflies notation are C_i, C_{2h}, C_{3i}, C_{4h}, C_{6h}, D_{2h}, D_{3d}, D_{4h}, D_{6h}, T_h and O_h, which has C_1, C_2, C_3, C_4, C_6, D_2, D_3, D_4, D_6, T, and O as their proper subgroup (e.g. $C_{2h} = C_2 \bigcup \boldsymbol{I}C_2$), respectively.

Improper crystallographic point groups that do not contain the inversion can be decomposed as the disjoint union of G_p and its coset $\bar{\boldsymbol{R}}G_p$, i.e., $G_i = G_p \bigcup \bar{\boldsymbol{R}}G_p$, where $\bar{\boldsymbol{R}} = \boldsymbol{IR}$ with $\boldsymbol{R} \notin G_p$ (otherwise $\bar{\boldsymbol{R}}\boldsymbol{R}^{-1} = \boldsymbol{IRR}^{-1} = \boldsymbol{I}$ which contradicts $\boldsymbol{I} \notin G_i$). To determine all such improper groups, we need the following theorem.

Theorem 2.1.2. [35] *Any improper group ($G_i = G_p \bigcup \bar{\boldsymbol{R}}G_p$) not containing the inversion is isomorphic to the proper group G' which can be written as $G' = G_p \bigcup \boldsymbol{R}G_p$ (where $\bar{\boldsymbol{R}} = \boldsymbol{IR}$ and $\boldsymbol{R} \notin G_p$).*

Proof. We just need to show $G' = G_p \bigcup \boldsymbol{R}G_p$ is indeed a group. It is clear that $\boldsymbol{E}$ is in G', and the elements of G' satisfy the associativity law because we have $(AB)C = A(BC)$ for matrix multiplications. Thus there remain two things to check: (1) there exists a unique inverse for each $a \in G'$ and (2) $ab \in G'$ for any a, $b \in G'$. Let $\boldsymbol{R}$, $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ be any elements in G_p and $\bar{\boldsymbol{R}} = \boldsymbol{IR}$. That $(\bar{\boldsymbol{R}}\boldsymbol{R}_1)^{-1} \in \bar{\boldsymbol{R}}G_p$ implies $(\boldsymbol{RR}_1)^{-1} \in \boldsymbol{R}G_p$ completes the proof of (1). To prove (2): First, if $a, b \in G_p$ (let $a = \boldsymbol{R}_1$ and $b = \boldsymbol{R}_2$), then clearly $ab = \boldsymbol{R}_1\boldsymbol{R}_2 \in G_p \subset G'$. Second, if $a = \boldsymbol{R}_1 \in G_p$ and $b = \boldsymbol{RR}_2 \in \boldsymbol{R}G_p$, then to show $ab = \boldsymbol{R}_1(\boldsymbol{RR}_2) \in \boldsymbol{R}G_p$, it suffices to show $\boldsymbol{R}_1(\boldsymbol{IRR}_2) = \boldsymbol{R}_1(\bar{\boldsymbol{R}}\boldsymbol{R}_2) \in \bar{\boldsymbol{R}}G_p \subset G_i$, which is trivial because $\boldsymbol{R}_1, (\bar{\boldsymbol{R}}\boldsymbol{R}_2) \in G_i$, which is a group. And we can get similar result if $a = \boldsymbol{RR}_1 \in \boldsymbol{R}G_p$ and $b = \boldsymbol{R}_2 \in G_p$. Last, if $a, b \in \boldsymbol{R}G_p$ with $a = \boldsymbol{RR}_1$ and $b = \boldsymbol{RR}_2$, then we also have $ab = (\boldsymbol{RR}_1)(\boldsymbol{RR}_2) \in G_p$. Indeed, $(\bar{\boldsymbol{R}}\boldsymbol{R}_1)(\bar{\boldsymbol{R}}\boldsymbol{R}_2) \in G_i$ and $\boldsymbol{R}, \boldsymbol{R}_1, \boldsymbol{R}_2 \in G_p$ imply $(\boldsymbol{IRR}_1)(\boldsymbol{IRR}_2) = (\boldsymbol{RR}_1)(\boldsymbol{RR}_2) \in G_p$. □

By this theorem, the proper groups that correspond to these improper groups have to be subgroups of index 2. Notice that the groups C_1, C_3, and T have no subgroup of index 2, while D_4 and D_6 each has two different subgroups of index 2. Hence we have $11-3+2 = 10$ new improper groups not containing the inversion, which in the Schönflies notation are C_s, C_{2v}, S_4, C_{4v}, D_{2d}, C_{3v}, C_{3h}, D_{3h}, C_{6v}, T_d.

In summary, there are 32 crystallographic point groups, which can be categorized in three types.

Type I: 11 rotational point groups, i.e., proper groups with $\det \boldsymbol{R} = 1$, namely,

$$C_1, C_2, C_3, C_4, C_6, D_2, D_3, D_4, D_6, T, O$$

Type II: 11 improper groups containing inversion, namely,

$$C_i, C_{2h}, C_{3i}, C_{4h}, C_{6h}, D_{2h}, D_{3d}, D_{4h}, D_{6h}, T_h, O_h$$

Type III: 10 improper groups not containing inversion, namely,

$$C_s, C_{2v}, S_4, C_{4v}, D_{2d}, C_{3v}, C_{3h}, D_{3h}, C_{6v}, T_d$$

Since most metals, with b.c.c, f.c.c, and h.c.p lattices (body centered cubic, face centered cubic, and hexagonal close packed, respectively), are centrosymmetric, Type II is especially important in texture analysis in metallurgy. The non-centrosymmetric crystal classes (Type I and III) are more important in mineralogical and geological problems.

2.1.3 Laue classes

When radiation and particles (e.g. electrons, neutrons, X-rays) interact with a crystal, it is impossible to distinguish by diffraction between crystals with symmetry defined by a centrosymmetric point group or one of its non-centrosymmetric subgroups. This is a consequence of Friedel's law, i.e., the diffraction pattern is always centrosymmetric regardless

Table 2.1: The 11 Laue classes

1.	C_1, C_i	7.	D_3, C_{3v}, D_{3d}
2.	C_2, C_s, C_{2h}	8.	D_4, C_{4v}, D_{2d}, D_{4h}
3.	C_3, C_{3i}	9.	D_6, C_{6v}, D_{3h}, D_{6h}
4.	C_4, S_4, C_{4h}	10.	T, T_h
5.	C_6, C_{3h}, C_{6h}	11.	O, T_d, O_h
6.	D_2, C_{2v}, D_{2h}		

of whether an inversion center is present in the crystal or not [7, 31]. This leads to another classification of crystallographic point groups, called Laue classes. The 32 crystallographic point groups can be divided into 11 Laue classes as in Table 2.1 and Table 2.2. Crystals with symmetry group in the same Laue class cannot be distinguished by diffraction techniques. The historical development of texture analysis might have followed a different route if during its formative years (1960s to 1980s) X-ray diffraction were not the only technique available for measurement of the ODF.

Table 2.2: Group structure in the same Laue class. For brevity, let $\boldsymbol{R}_1 = \boldsymbol{R}(e_3, \pi)$, $\boldsymbol{R}_2 = \boldsymbol{R}(e_3, \frac{\pi}{2})$, $\boldsymbol{R}_3 = \boldsymbol{R}(e_3, \frac{\pi}{3})$ and $\boldsymbol{R}_4 = \boldsymbol{R}(e_2, \pi)$.

Laue Classes	Type I	Type II	Type III
1. C_1, C_i	C_1	$C_i = C_1 \cup \boldsymbol{I}C_1$	
2. C_2, C_{2h}, C_s	$C_2 = C_1 \cup \boldsymbol{R}_1 C_1$	$C_{2h} = C_2 \cup \boldsymbol{I}C_2$	$C_s = C_1 \cup \boldsymbol{I}\boldsymbol{R}_1 C_1$
3. C_3, C_{3i}	C_3	$C_{3i} = C_3 \cup \boldsymbol{I}C_3$	
4. C_4, C_{4h}, S_4	$C_4 = C_2 \cup \boldsymbol{R}_2 C_2$	$C_{4h} = C_4 \cup \boldsymbol{I}C_4$	$S_4 = C_2 \cup \boldsymbol{I}\boldsymbol{R}_2 C_2$
5. C_6, C_{6h}, C_{3h}	$C_6 = C_3 \cup \boldsymbol{R}_3 C_3$	$C_{6h} = C_6 \cup \boldsymbol{I}C_6$	$C_{3h} = C_3 \cup \boldsymbol{I}\boldsymbol{R}_3 C_3$
6. D_2, D_{2h}, C_{2v}	$D_2 = C_2 \cup \boldsymbol{R}_4 C_2$	$D_{2h} = D_2 \cup \boldsymbol{I}D_2$	$C_{2v} = C_2 \cup \boldsymbol{I}\boldsymbol{R}_4 C_2$
7. D_3, D_{3d}, C_{3v}	$D_3 = C_3 \cup \boldsymbol{R}_4 C_3$	$D_{3d} = D_3 \cup \boldsymbol{I}D_3$	$C_{3v} = C_3 \cup \boldsymbol{I}\boldsymbol{R}_4 C_3$
8. D_4, D_{4h} , C_{4v} 8. D_4, D_{2d}	$D_4 = C_4 \cup \boldsymbol{R}_4 C_4$ $D_4 = D_2 \cup \boldsymbol{R}_2 D_2$	$D_{4h} = D_4 \cup \boldsymbol{I}D_4$	$C_{4v} = C_4 \cup \boldsymbol{I}\boldsymbol{R}_4 C_4$ $D_{2d} = D_2 \cup \boldsymbol{I}\boldsymbol{R}_2 D_2$
9. D_6, D_{6h}, D_{3h} 9. D_6, C_{6v}	$D_6 = D_3 \cup \boldsymbol{R}_3 D_3$ $D_6 = C_6 \cup \boldsymbol{R}_4 C_6$	$D_{6h} = D_6 \cup \boldsymbol{I}D_6$	$D_{3h} = D_3 \cup \boldsymbol{I}\boldsymbol{R}_3 D_3$ $C_{6v} = C_6 \cup \boldsymbol{I}\boldsymbol{R}_4 C_6$
10. T, T_h	T	$T_h = T \cup \boldsymbol{I}T$	
11. O, T_d, O_h	$O = T \cup \boldsymbol{R}_2 T$	$O_h = O \cup \boldsymbol{I}O$	$T_d = T \cup \boldsymbol{I}\boldsymbol{R}_2 T$

2.2 Basics of integration on O(3)

Much of the exposition that follows until the end of subsection 2.2.2 is adapted from the lecture notes of Man [18].

In classical texture analysis, the orientation of the crystal lattice $L(X)$ at a sampling point X in a polycrystal is defined by the rotation $\boldsymbol{R}(X)$ that takes the lattice L_{ref} of an arbitrarily-chosen reference single crystal to $L(X)$. It is assumed that a probability distribution function $w : \text{SO}(3) \to \mathbb{R}^1$, called the orientation distribution function (ODF), can be defined so that

$$\int_{\mathcal{A}} w(\boldsymbol{R})\, d\mathcal{V},$$

where $\mathcal{V}$ is a suitable positive ("volume") measure on SO(3) and $\mathcal{A} \subset \text{SO}(3)$, gives the probability of finding $\boldsymbol{R}(X) \in \mathcal{A}$. In particular, the normalization condition

$$\int_{\text{SO}(3)} w(\boldsymbol{R})\, d\mathcal{V} = 1 \tag{2.1}$$

should hold. To cover the possibility of macroscopic isotropy, where all orientations have the same probability or $w(\boldsymbol{R})$ = constant, we see from (2.1) that $\mathcal{V}$ must be a finite measure. Further physical considerations [18]—which concern the effects of sample rotations and the arbitrariness of the reference orientation on the ODF—dictate that the volume measure $\mathcal{V}$ should be left-invariant and right-invariant, i.e.

$$\mathcal{V}(\boldsymbol{R}\mathcal{A}) = \mathcal{V}(\mathcal{A}) \quad \text{and} \quad \mathcal{V}(\mathcal{A}\boldsymbol{R}) = \mathcal{V}(\mathcal{A}) \qquad \text{for any } \boldsymbol{R} \in \text{SO}(3). \tag{2.2}$$

In the present study, we will let ODFs to be defined on O(3) instead of SO(3), and our theory will subsume that of classical texture analysis. We will require the volume measure $\mathcal{V}$ on O(3) likewise to be finite, left-invariant, and right-invariant.

The rotation group SO(3) and the orthogonal group O(3) are compact topological groups. It is well known that on every compact topological group there exists a regular Borel measure, unique up to a positive multiplicative constant, which is finite, left-invariant, and right-invariant (see, e.g., Rudin [36]). Such measures are called Haar measures. For a given compact group, the normalized Haar measure (under which the group in question has unit measure) is unique. In what follows we shall determine the normalized Haar measure for SO(3) and for O(3), respectively, by using the fact that SO(3) and O(3) are Riemannian manifolds with a bi-invariant metric.

2.2.1 Geometric Structure of O(3)

Let V be the translation space of the three-dimensional physical Euclidean space, and let Lin be the space of linear transformations on V. We adopt and fix a right-handed orthonormal basis $\{\boldsymbol{e}_i\}$ ($i = 1, 2, 3$) of V, under which each linear transformation in Lin is represented by a matrix in M(3), the space of 3×3 real matrices. In what follows we shall identify each linear transformation $\boldsymbol{A}$ in Lin with its representative in M(3), which we denote by the same symbol $\boldsymbol{A}$.

We equip M(3) with the inner product defined by

$$\boldsymbol{A} \cdot \boldsymbol{B} = \frac{1}{2}\mathrm{tr}(\boldsymbol{A}\boldsymbol{B}^T) \qquad \text{for } \boldsymbol{A}, \boldsymbol{B} \in \mathrm{M}(3). \tag{2.3}$$

We choose and fix an orthonormal basis $\boldsymbol{E}_i$ ($i = 1, 2, ..., 9$) in M(3) as follows. Let

$$\boldsymbol{E}_1 = -\boldsymbol{e}_2 \otimes \boldsymbol{e}_3 + \boldsymbol{e}_3 \otimes \boldsymbol{e}_2, \quad \boldsymbol{E}_2 = -\boldsymbol{e}_3 \otimes \boldsymbol{e}_1 + \boldsymbol{e}_1 \otimes \boldsymbol{e}_3, \quad \boldsymbol{E}_3 = -\boldsymbol{e}_1 \otimes \boldsymbol{e}_2 + \boldsymbol{e}_2 \otimes \boldsymbol{e}_1,$$
$$\boldsymbol{E}_4 = \sqrt{2}(\boldsymbol{e}_1 \otimes \boldsymbol{e}_1), \quad \boldsymbol{E}_5 = \sqrt{2}(\boldsymbol{e}_2 \otimes \boldsymbol{e}_2), \quad \boldsymbol{E}_6 = \sqrt{2}(\boldsymbol{e}_3 \otimes \boldsymbol{e}_3),$$
$$\boldsymbol{E}_7 = \boldsymbol{e}_2 \otimes \boldsymbol{e}_3 + \boldsymbol{e}_3 \otimes \boldsymbol{e}_2, \quad \boldsymbol{E}_8 = \boldsymbol{e}_3 \otimes \boldsymbol{e}_1 + \boldsymbol{e}_1 \otimes \boldsymbol{e}_3, \quad \boldsymbol{E}_9 = \boldsymbol{e}_1 \otimes \boldsymbol{e}_2 + \boldsymbol{e}_2 \otimes \boldsymbol{e}_1.$$

It is easy to verify that under the inner product (2.3) the matrices $\boldsymbol{E}_i$ ($i = 1, 2, ..., 9$) constitute an orthonormal basis in M(3). Every $\boldsymbol{X} \in \mathrm{M}(3)$ can be written uniquely as a linear combination $\boldsymbol{X} = \sum_i X_i \boldsymbol{E}_i$, where $X_i \in \mathbb{R}^1$ for each i. Let $\varphi : \mathrm{M}(3) \to \mathbb{R}^9$ be defined by

$$\varphi(\sum_i X_i \boldsymbol{E}_i) = (X_1, X_2, ..., X_9). \tag{2.4}$$

The function φ, which is clearly a homeomorphism between M(3) and $\mathbb{R}^9$, defines a global chart on M(3) and a C^∞ differentiable structure there. It is easy to show that this differentiable structure is independent of the basis chosen in M(3). We take GL(3), the set of non-singular 3×3 matrices, as an open submanifold of M(3), and endow the subspaces Sym (the space of symmetric matrices) and Skw (the space of skew-symmetric matrices) each with the differentiable structure that make them embedded submanifolds of M(3).

It is easy to show that both the orthogonal group

$$\mathrm{O}(3) = \{\boldsymbol{Q} \in \mathrm{M}(3) : \boldsymbol{Q}\boldsymbol{Q}^T = \boldsymbol{E}\} \tag{2.5}$$

and the rotation group

$$\mathrm{SO}(3) = \{\boldsymbol{Q} \in \mathrm{M}(3) : \boldsymbol{Q}\boldsymbol{Q}^T = \boldsymbol{E} \text{ and } \det \boldsymbol{Q} = 1\} \tag{2.6}$$

are 3-dimensional embedded submanifolds of M(3) [14]. Let $\Psi : \mathrm{M}(3) \to \mathrm{Sym}$ be the function defined by

$$\Psi(\boldsymbol{A}) = \boldsymbol{A}\boldsymbol{A}^T. \tag{2.7}$$

It is clear that Ψ is of class C^∞ and that $\Psi^{-1}(\boldsymbol{E}) = \mathrm{O}(3)$. Since O(3) is a level set of the continuous function Ψ, it is a closed subset of M(3). Moreover, O(3) is bounded in M(3) because $\|\boldsymbol{Q}\| = \sqrt{3}$ for each $\boldsymbol{Q} \in \mathrm{O}(3)$. Hence O(3) is compact.

Each $\boldsymbol{Q} \in \mathrm{O}(3)$ is orthogonal. Thus $\det \boldsymbol{Q}$ satisfies

$$(\det \boldsymbol{Q})^2 = (\det \boldsymbol{Q})(\det \boldsymbol{Q}^T) = \det(\boldsymbol{Q}\boldsymbol{Q}^T) = \det \boldsymbol{E} = 1,$$

which implies $\det \boldsymbol{Q} = \pm 1$. If $\det \boldsymbol{Q} = 1$, then $\boldsymbol{Q} = \boldsymbol{R}$ for some $\boldsymbol{R} \in \mathrm{SO}(3)$. If $\det \boldsymbol{Q} = -1$, then $\det(\boldsymbol{I}\boldsymbol{Q}) = 1$ and there is an $\boldsymbol{R} \in \mathrm{SO}(3)$ such that $\boldsymbol{I}\boldsymbol{Q} = \boldsymbol{R}$ or $\boldsymbol{Q} = \boldsymbol{I}\boldsymbol{R}$. Since the map $h : \mathrm{O}(3) \to \mathbb{R}^1$, $\boldsymbol{Q} \mapsto \det \boldsymbol{Q}$, is continuous, O(3) is the disjoint union of $\mathcal{G} := \mathrm{SO}(3)$ and

$$\boldsymbol{I}\mathcal{G} := \{\boldsymbol{I}\boldsymbol{R} : \boldsymbol{R} \in \mathrm{SO}(3)\}. \tag{2.8}$$

As a closed and open subset of O(3), SO(3) is compact and is an embedded submanifold of M(3).

For each $\boldsymbol{A} \in$ M(3), $T_{\boldsymbol{A}}M(3)$—the tangent space to M(3) at $\boldsymbol{A}$—can be identified with M(3), which carries the inner product (2.3). Hence M(3) is a Riemannian manifold. As embedded submanifolds of M(3), both O(3) and SO(3) are Riemannian. For each $\boldsymbol{Q} \in$ O(3), $T_{\boldsymbol{Q}}O(3)$ is a linear subspace of $T_{\boldsymbol{Q}}M(3)$ and carries the inner produce induced by that of M(3), namely (2.3). A similar statement holds for the tangent spaces to SO(3).

Before we close this subsection, we characterize the structure of the tangent spaces $T_{\boldsymbol{Q}}\mathrm{O}(3)$, where $\boldsymbol{Q} \in$ O(3). Consider a smooth curve $\boldsymbol{B}(t)$ in O(3) that passes through the element $\boldsymbol{Q}$ at $t = 0$, i.e., $\boldsymbol{B}(0) = \boldsymbol{Q}$. Then $\boldsymbol{A}(t) := \boldsymbol{Q}^T\boldsymbol{B}(t)$ defines a smooth curve in O(3) that satisfies $\boldsymbol{A}(0) = \boldsymbol{E}$. Differentiating both sides of the equation $\boldsymbol{A}(t)\boldsymbol{A}(t)^T = \boldsymbol{E}$ and then setting $t = 0$, we obtain

$$\dot{\boldsymbol{A}}(0)\boldsymbol{A}(0)^T + \boldsymbol{A}(0)\dot{\boldsymbol{A}}(0)^T = \boldsymbol{0},$$

which implies $\dot{\boldsymbol{A}}(0) = -\dot{\boldsymbol{A}}(0)^T$ or $\boldsymbol{Q}^T\dot{\boldsymbol{B}}(0)$ is skew. Thus there exists a skew matrix $\boldsymbol{W}$ such that the tangent vector $\dot{\boldsymbol{B}}(0) \in T_{\boldsymbol{Q}}\mathrm{O}(3)$ is given by $\dot{\boldsymbol{B}}(0) = \boldsymbol{Q}\boldsymbol{W}$. Conversely, for each $\boldsymbol{W} \in$ Skw, $\boldsymbol{C}(t) := \boldsymbol{Q}\exp(t\boldsymbol{W})$ defines a smooth curve in O(3) that satisfies $\boldsymbol{C}(0) = \boldsymbol{Q}$ and $\dot{\boldsymbol{C}}(0) = \boldsymbol{Q}\boldsymbol{W}$ is a tangent vector in $T_{\boldsymbol{Q}}\mathrm{O}(3)$. We conclude that

$$T_{\boldsymbol{Q}}\mathrm{O}(3) = \{\boldsymbol{Q}\boldsymbol{W} : \boldsymbol{W} \in \mathrm{Skw}\}. \tag{2.9}$$

In particular, $T_{\boldsymbol{E}}\mathrm{O}(3)$ is none other than the space of skew tensors Skw.

2.2.2 Bi-invariant Metric

A smooth manifold G is a Lie group if the following two assertions hold:

1. G is a group.

2. The group operations $G \times G \to G$, $(x, y) \mapsto xy$ and $G \to G$, $x \mapsto x^{-1}$ are smooth functions.

For each $a \in G$, we define the left translation $L_a : G \to G$ and right translation $R_a : G \to G$ by

$$L_a(x) = ax \qquad \text{for each } x \in G, \tag{2.10}$$

and

$$R_a(x) = xa \qquad \text{for each } x \in G, \tag{2.11}$$

respectively. It is clear that both L_a and R_a are smooth functions. The groups GL(3), O(3), and SO(3) are examples of Lie groups.

Let G be a Lie group and a Riemannian manifold. Let $<u, v>_x$ denote the inner product of tangent vectors u, v in T_xG. The Riemannian metric on G is said to be left-invariant if each left-translation on G is an isometry, i.e.,

$$<u, v>_x = <DL_a(x)[u], DL_a(x)[v]>_{L_a(x)} \qquad \text{for all } a, x \in G \text{ and } u, v \in T_xG, \tag{2.12}$$

and right-invariant if each right-translation is an isometry. A Riemannian metric is bi-invariant if it is both left-invariant and right-invariant.

In what follows we show that the Riemannian metric on O(3) is bi-invariant. For a given $\boldsymbol{A} \in$ O(3), we have by definition (2.10)

$$L_{\boldsymbol{A}}(\boldsymbol{Q}) = \boldsymbol{AQ} \qquad \text{for each } \boldsymbol{Q} \in \mathrm{O}(3). \tag{2.13}$$

Let $\boldsymbol{W}$ be skew and let $\boldsymbol{QW}$ be a tangent vector in $T_{\boldsymbol{Q}}$O(3). It is easy to verify that

$$DL_{\boldsymbol{A}}(\boldsymbol{Q})[\boldsymbol{QW}] = \boldsymbol{AQW}. \tag{2.14}$$

To verify that the Riemannian metric on O(3) is left-invariant, we have to check that requirement (2.12) is observed. Let $\boldsymbol{A}$, $\boldsymbol{Q}$ be in O(3), and let $\boldsymbol{X}$ and $\boldsymbol{Y}$ be skew. On the left-hand side of requirement (2.12), we have

$$<\boldsymbol{QX}, \boldsymbol{QY}>_{\boldsymbol{Q}} = \frac{1}{2}\mathrm{tr}\left(\boldsymbol{QX}(\boldsymbol{QY})^T\right) = \frac{1}{2}\mathrm{tr}\left(\boldsymbol{XY}^T\right).$$

On the right-hand side, there holds

$$\begin{aligned} <DL_{\boldsymbol{A}}(\boldsymbol{Q})[\boldsymbol{QX}], DL_{\boldsymbol{A}}(\boldsymbol{Q})[\boldsymbol{QY}]>_{L_{\boldsymbol{A}}(\boldsymbol{Q})} &= \frac{1}{2}\mathrm{tr}\left(\boldsymbol{AQX}(\boldsymbol{AQY})^T\right) \\ &= \frac{1}{2}\mathrm{tr}\left(\boldsymbol{XY}^T\right). \end{aligned}$$

Hence the Riemannian metric on O(3) is left-invariant. That it is also right-invariant can be proved in a similar way. In conclusion, the Riemannian metric on O(3) is bi-invariant.

Similarly the Riemannian metric on SO(3) is also bi-invariant.

2.2.3 Integration on O(3)

By the discussions in the previous two subsections, we can determine the (normalized) Haar measure on O(3) by computing the volume element pertaining to the invariant metric on the Lie group.

All rotations $\boldsymbol{R}$ that satisfy $\boldsymbol{Re}_3 \neq \boldsymbol{e}_3$ can be parametrized by the Euler angles (ψ, θ, ϕ), where $0 \leq \phi < 2\pi$, $0 < \theta < \pi$, and $0 \leq \phi < 2\pi$. For these $\boldsymbol{R} \in$ SO(3), we can write $\boldsymbol{R}(\psi, \theta, \phi) = \boldsymbol{R}(e_3, \psi)\boldsymbol{R}(e_2, \theta)\boldsymbol{R}(e_3, \phi)$ [18, 26]. For any element in $\boldsymbol{I}$SO(3), we can write it as $\boldsymbol{IR}(\psi, \theta, \phi)$. For brevity, let $\boldsymbol{R} = \boldsymbol{R}(\psi, \theta, \phi)$, $\boldsymbol{R}_1 = \boldsymbol{R}(e_3, \psi)$, $\boldsymbol{R}_2 = \boldsymbol{R}(e_2, \theta)$ and $\boldsymbol{R}_3 = \boldsymbol{R}(e_3, \phi)$. The matrix expressions are given as following.

$$\boldsymbol{R}_1 = \begin{pmatrix} \cos(\psi) & -\sin(\psi) & 0 \\ \sin(\psi) & \cos(\psi) & 0 \\ 0 & 0 & 1 \end{pmatrix}; \tag{2.15}$$

$$\boldsymbol{R}_2 = \begin{pmatrix} \cos(\theta) & 0 & \sin(\theta) \\ 0 & 1 & 0 \\ -\sin(\theta) & 0 & \cos(\theta) \end{pmatrix}; \tag{2.16}$$

$$\boldsymbol{R}_3 = \begin{pmatrix} \cos(\phi) & -\sin(\phi) & 0 \\ \sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & 1 \end{pmatrix}; \tag{2.17}$$

and

$$\boldsymbol{R} = \begin{pmatrix} \cos(\psi)\cos(\theta)\cos(\phi) - \sin(\psi)\sin(\phi) & -\cos(\psi)\cos(\theta)\sin(\phi) - \sin(\psi)\cos(\phi) & \cos(\psi)\sin(\theta) \\ \sin(\psi)\cos(\theta)\cos(\phi) + \cos(\psi)\sin(\phi) & -\sin(\psi)\cos(\theta)\sin(\phi) + \cos(\psi)\cos(\phi) & \sin(\psi)\sin(\theta) \\ -\sin(\theta)\cos(\phi) & \sin(\theta)\sin(\phi) & \cos(\theta) \end{pmatrix}. \tag{2.18}$$

Now we can write $\boldsymbol{R} = \boldsymbol{R}_1\boldsymbol{R}_2\boldsymbol{R}_3 = e^{\psi \boldsymbol{E}_3} e^{\theta \boldsymbol{E}_2} e^{\phi \boldsymbol{E}_3}$ [18]. The formula of components of the Riemannian metric tensor in local coordinates ψ, θ, ϕ is given as $g_{ij} = < \frac{\partial \boldsymbol{R}}{\partial x_i}, \frac{\partial \boldsymbol{R}}{\partial x_j} >$, where $x_1 = \psi$, $x_2 = \theta$, and $x_3 = \phi$ [13, 25]. For example,

$$\begin{aligned}
g_{11} &= < \frac{\partial \boldsymbol{R}}{\partial \psi}, \frac{\partial \boldsymbol{R}}{\partial \psi} > = < \frac{\partial (e^{\psi \boldsymbol{E}_3} e^{\theta \boldsymbol{E}_2} e^{\phi \boldsymbol{E}_3})}{\partial \psi}, \frac{\partial (e^{\psi \boldsymbol{E}_3} e^{\theta \boldsymbol{E}_2} e^{\phi \boldsymbol{E}_3})}{\partial \psi} > \\
&= < e^{\psi \boldsymbol{E}_3} \boldsymbol{E}_3 e^{\theta \boldsymbol{E}_2} e^{\phi \boldsymbol{E}_3}, e^{\psi \boldsymbol{E}_3} \boldsymbol{E}_3 e^{\theta \boldsymbol{E}_2} e^{\phi \boldsymbol{E}_3} > = < \boldsymbol{R}_1 \boldsymbol{E}_3 \boldsymbol{R}_2 \boldsymbol{R}_3, \boldsymbol{R}_1 \boldsymbol{E}_3 \boldsymbol{R}_2 \boldsymbol{R}_3 > \\
&= \frac{1}{2} \mathrm{tr}(\boldsymbol{R}_1 \boldsymbol{E}_3 \boldsymbol{R}_2 \boldsymbol{R}_3 (\boldsymbol{R}_1 \boldsymbol{E}_3 \boldsymbol{R}_2 \boldsymbol{R}_3)^T) = \frac{1}{2} \mathrm{tr}(\boldsymbol{R}_1 \boldsymbol{E}_3 \boldsymbol{R}_2 \boldsymbol{R}_3 \boldsymbol{R}_3^T \boldsymbol{R}_2^T \boldsymbol{E}_3^T \boldsymbol{R}_1^T) \\
&= \frac{1}{2} \mathrm{tr}(\boldsymbol{R}_1 \boldsymbol{E}_3 \boldsymbol{E}_3^T \boldsymbol{R}_1^T) = \frac{1}{2} \mathrm{tr}(\boldsymbol{R}_1 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \boldsymbol{R}_1^T) = \frac{1}{2} \mathrm{tr}(\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \boldsymbol{R}_1 \boldsymbol{R}_1^T) \\
&= \frac{1}{2} \mathrm{tr}(\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}) = 1,
\end{aligned} \tag{2.19}$$

where we have used the fact that $\boldsymbol{R}_i\boldsymbol{R}_i^T = \boldsymbol{E}$ for $i = 1, 2, 3$ and

$$\boldsymbol{E}_3\boldsymbol{E}_3^T = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The author computed the other components by writing a short Maple program (see Appendix 1). In summary, the matrix representation (g_{ij}) of the metric tensor in question is:

$$(g_{ij}) = \begin{pmatrix} 1 & 0 & \cos\theta \\ 0 & 1 & 0 \\ \cos\theta & 0 & 1 \end{pmatrix}. \tag{2.20}$$

Thus the volume element is $\sqrt{\det(g_{ij})} = \sin\theta$ and the volume of SO(3) is:

$$\mathcal{V}(\mathrm{SO}(3)) = \int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} w(\boldsymbol{R}(\psi, \theta, \phi)) \sin\theta \, d\psi d\theta d\phi = 8\pi^2. \tag{2.21}$$

Hence the normalized Haar measure g of a Borel set $\mathcal{A}$ in SO(3) is:

$$g(\mathcal{A}) = \int_{\mathrm{SO}(3)} \chi_{\mathcal{A}} \, dg = \frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} \chi_{\mathcal{A}} \sin\theta \, d\psi d\theta d\phi, \tag{2.22}$$

where $\chi_{\mathcal{A}}$ is the characteristic function of $\mathcal{A}$ defined by

$$\chi_{\mathcal{A}}(x) = \begin{cases} 1 & \text{if } x \in \mathcal{A} \\ 0 & \text{if } x \notin \mathcal{A} \end{cases}.$$

In line with Roe's pioneering work [32] in texture analysis, we will give SO(3) the volume measure $\mathcal{V} = 8\pi^2 g$.

Since O(3) is the disjoint union of SO(3) and $\boldsymbol{I}$SO(3), both of which are Riemannian submanifolds of M(3) and are isometric under the mapping SO(3) → $\boldsymbol{I}$SO(3), $\boldsymbol{R} \mapsto \boldsymbol{IR}$, we give $\boldsymbol{I}$SO(3) the volume measure that, for every measurable set $\mathcal{A} \subset$ SO(3), the volume of $\boldsymbol{I}\mathcal{A}$ is the same as that of $\mathcal{A}$, i.e., $\mathcal{V}(\mathcal{A})$. As no confusion should arise, we denote this measure on $\boldsymbol{I}$SO(3) and the consequent volume measure on O(3) all by $\mathcal{V}$. Then we have

$$\mathcal{V}(\mathrm{O}(3)) = 2\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} w(\boldsymbol{R}(\psi,\theta,\phi))\sin\theta\, d\psi d\theta d\phi = 16\pi^2. \tag{2.23}$$

For $\mathcal{A} = \mathcal{A}_1 \cup \mathcal{A}_2$ in O(3), where $\mathcal{A}_1 \subset$ SO(3) and $\mathcal{A}_2 \subset \boldsymbol{I}$SO(3) are Borel sets, the normalized Haar measure of $\mathcal{A}$ is:

$$\int_{\mathrm{O}(3)} \chi_{\mathcal{A}}\, dg = \frac{1}{16\pi^2}\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} \chi_{\mathcal{A}_1}\sin\theta\, d\psi d\theta d\phi + \frac{1}{16\pi^2}\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} \chi_{\mathcal{A}_2}\sin\theta\, d\psi d\theta d\phi. \tag{2.24}$$

In what follows there will be occasions that we use the axis-angle parametrization of rotations in integrations. Under the axis-angle parametrization, a rotation $\boldsymbol{R}$ is specified by the direction $\boldsymbol{n}(\Theta, \Phi)$ of its axis, where $(1, \Theta, \Phi)$ are the spherical coordinates of $\boldsymbol{n}$, and the angle of rotation $0 < \omega < \pi$. Note that the ranges of Θ and Φ are $0 < \Theta < \pi$, $0 \leq \Phi < 2\pi$. It can be shown [18, 40] that

$$\sin\theta\, d\phi d\theta d\phi = 4\sin^2\frac{\omega}{2}\sin\Theta\, d\omega d\Theta d\Phi \tag{2.25}$$

on SO(3).

2.3 Group representations

2.3.1 Basics of group representations

Definition 2.3.1. [28] *Let G be a group and let X be a complex linear space ($\neq \{0\}$). Consider a mapping T of G into the set of all linear operators carrying X into itself, written $g \mapsto T(g)$, with the following properties:*

1. $T(e) = 1$, *where e is the identity of G and 1 is the identity operator in X;*

2. $T(g_1 g_2) = T(g_1)T(g_2)$ *for all $g_1, g_2 \in G$.*

Then T is called a representation of G in the space X. The space X is called the representation space and the operators $T(g)$ representation operators.

Remark: Let $\dim X < +\infty$, and let $\mathrm{GL}(X)$ be the space of non-singular linear transformations on X. Then a homomorphism

$$T : G \to \mathrm{GL}(X)$$

is a representation of G on X.

Two representations T, S of a group G in spaces X and Y are called equivalent if there is a one-to-one linear operator A carrying X onto Y and satisfying the condition $AT(g) = S(g)A$, for all $g \in G$. It is possible that $X = Y$, and in this case we speak of the equivalence of the representation in the same space. For the case where X and Y are finite-dimensional, representations S and T on X and Y are equivalent representations if and only if $n_S = n_T$ (dimensions of S and T) and under a proper choice of bases in X and Y, the matrix which represents S coincides with that which represents T [28].

A representation T of G in a pre-Hilbert space X (a linear space with a scalar product) is called unitary if all operators of the representation are unitary, i.e., $\langle Ax, Ay\rangle = \langle x, y\rangle$ [28]. In what follows we recall the definition of Hermitian inner product.

Definition 2.3.2. [38] *A Hermitian inner product on a complex vector space V is a complex-valued bilinear form on V which is antilinear in the second slot, and is positive definite. That is, it satisfies the following properties, where $\overline{z}$ denotes the complex conjugate of z.*

1. $\langle x + y, z\rangle = \langle x, z\rangle + \langle y, z\rangle$ *and* $\langle x, y + z\rangle = \langle x, y\rangle + \langle x, z\rangle$

2. $\langle ax, y\rangle = a\langle x, y\rangle$ *and* $\langle x, ay\rangle = \overline{a}\langle x, y\rangle$

3. $\langle x, y\rangle = \overline{\langle y, x\rangle}$

4. $\langle x, x\rangle \geq 0$*, with equality only if* $x = 0$

Note the inner product defines a metric topology on X by $d(x,y) = \sqrt{\langle x-y, x-y\rangle}$. A basic example is the form $\langle x, y\rangle = \sum_{i=1}^{n} x_i\overline{y_i}$ in $\mathbb{C}^n$.

A representation T of G in X is said to be (strongly) continuous if $g \mapsto T(g)x$ is continuous on G for every $x \in X$. A subspace $M \subset X$ is said to be invariant under a representation T if it is invariant under all operators $T(g)$ of this representation. A representation in a space X is called irreducible if, except for $\{0\}$ and X itself, the space X admits no subspace invariant under the representation. A set $\{T_\alpha\}$ of representations of the group G is called a complete set of irreducible representations of G if (i) the representations T_α are irreducible and are pairwise inequivalent, and (ii) every irreducible representation of G is equivalent to one of the representations T_α [28].

2.3.2 Irreducible representations of SO(3)

The rotation group SO(3) has a complete set of pairwise-inequivalent, strongly continuous, irreducible unitary representations $\mathcal{D}_l$ $(l = 0, 1, 2, \cdots)$ of dimension $2l + 1$ [20, 38], which can be defined by means of the Wigner D-functions $D^l_{mn} : \mathrm{SO}(3) \to \mathbb{C}$, with $\mathcal{D}_l : \boldsymbol{R} \mapsto [D^l_{mn}(\boldsymbol{R})]$, where $[D^l_{mn}(\boldsymbol{R})]$ denotes the $(2l+1)\times(2l+1)$ matrix with entries $D^l_{mn}(\boldsymbol{R})$ $(-l \leq m \leq l, -l \leq n \leq l)$.

The Wigner D-functions are given by the following formulas [18, 20, 40].

$$D^l_{mn}(\boldsymbol{R}(\psi,\theta,\phi)) = d^l_{mn}(\theta)e^{-i(m\psi+n\phi)}, \tag{2.26}$$

where

$$d^l_{mn}(\theta) = \sum_{k=\max\{m-n,\,0\}}^{\min\{l-n,\,l+m\}} \frac{(-1)^k\sqrt{(l+m)!(l-m)!(l+n)!(l-n)!}}{k!(l-n-k)!(l+m-k)!(k-m+n)!} \times \left(\cos\frac{\theta}{2}\right)^{2l-n+m-2k}\left(\sin\frac{\theta}{2}\right)^{2k-m+n}. \tag{2.27}$$

and the Wigner D-functions satisfy the identities

$$D^l_{mn}(\boldsymbol{R}_1\boldsymbol{R}_2) = \sum_{p=-l}^{l} D^l_{mp}(\boldsymbol{R}_1)D^l_{pn}(\boldsymbol{R}_2), \tag{2.28}$$

$$D^l_{mn}(\boldsymbol{R}^{-1}) = \overline{D^l_{nm}(\boldsymbol{R})} \tag{2.29}$$

for all rotations $\boldsymbol{R}, \boldsymbol{R}_1, \boldsymbol{R}_2 \in \mathrm{SO}(3), l = 0, 1, 2, \cdots, -l \le m \le l$, and $-l \le n \le l$.

2.4 Material tensors and pseudotensors

2.4.1 Tensors and pseudotensors

Let V be the translation space of the three-dimensional physical space E^3, and let $V^r = V \times \cdots \times V$ (r copies), where $r \ge 2$. A mapping $\boldsymbol{H} : V^r \to \mathbb{R}^1$ is multilinear if it is linear with respect to each of its vector arguments, i.e.,

$$\boldsymbol{H}[\boldsymbol{v}_1, \cdots, \boldsymbol{v}_i + \alpha\boldsymbol{v}'_i, \cdots, \boldsymbol{v}_r] = \boldsymbol{H}[\boldsymbol{v}_1, \cdots, \boldsymbol{v}_i, \cdots, \boldsymbol{v}_r] + \alpha\boldsymbol{H}[\boldsymbol{v}_1, \cdots, \boldsymbol{v}'_i, \cdots, \boldsymbol{v}_r] \tag{2.30}$$

for each $\boldsymbol{v}_i$ ($1 \le i \le r$), $\boldsymbol{v}'_i \in V$ and $\alpha \in \mathbb{R}^1$. In mathematics such multilinear mappings are called rth-order tensors.[①] Let $\boldsymbol{u}_1, \cdots, \boldsymbol{u}_r$ be in V. The tensor product of $\boldsymbol{u}_1, \cdots, \boldsymbol{u}_r$ is the rth-order tensor $\boldsymbol{u}_1 \otimes \cdots \otimes \boldsymbol{u}_r : V^r \to \mathbb{R}^1$ defined by

$$\boldsymbol{u}_1 \otimes \cdots \otimes \boldsymbol{u}_r[\boldsymbol{v}_1, \cdots, \boldsymbol{v}_r] = (\boldsymbol{u}_1 \cdot \boldsymbol{v}_1) \cdots (\boldsymbol{u}_r \cdot \boldsymbol{v}_r) \quad \text{for each } (\boldsymbol{v}_1, \cdots, \boldsymbol{v}_r) \in V^r. \tag{2.31}$$

We call tensor products of vectors simple tensors. Under the usual definition of addition and of scalar multiplication of mappings, the set of rth-order tensors clearly forms a linear space over $\mathbb{R}^1$, which we denote by $V^{\otimes r} := V \otimes \cdots \otimes V$ (r copies) and call the space of rth-order tensors.

Let $\boldsymbol{e}_1$, $\boldsymbol{e}_2$, and $\boldsymbol{e}_3$ constitute a right-handed orthonormal basis in V. It is easy to see that every $\boldsymbol{H} \in V^{\otimes r}$ can be written in the form

$$\boldsymbol{H} = H_{i_1 i_2 \cdots i_r}\boldsymbol{e}_{i_1} \otimes \boldsymbol{e}_{i_2} \otimes \cdots \otimes \boldsymbol{e}_{i_r} \tag{2.32}$$

[①] In what follows we use the word "tensor" in two senses: (i) a multilinear mapping as defined in (2.30) for some $r \ge 2$; (ii) as in "material tensor", a multilinear mapping in the preceding sense that further obeys the law of transformation (2.38).

where the Einstein summation convention is in force and

$$H_{i_1 i_2 \cdots i_r} = \boldsymbol{H}[\boldsymbol{e}_{i_1}, \boldsymbol{e}_{i_2}, \cdots, \boldsymbol{e}_{i_r}]. \tag{2.33}$$

We define an inner product $<\cdot,\cdot>$ on $V^{\otimes r}$ by requiring that

$$<\boldsymbol{u}_1 \otimes \cdots \otimes \boldsymbol{u}_r, \boldsymbol{w}_1 \otimes \cdots \otimes \boldsymbol{w}_r> = (\boldsymbol{u}_1 \cdot \boldsymbol{w}_1) \cdots (\boldsymbol{u}_r \cdot \boldsymbol{w}_r). \tag{2.34}$$

Clearly simple tensors of the form $\boldsymbol{e}_{i_1} \otimes \boldsymbol{e}_{i_2} \otimes \cdots \otimes \boldsymbol{e}_{i_r}$, where each suffix runs over the indices 1, 2, and 3, constitute an orthonormal basis in $V^{\otimes r}$. Hence $\dim V^{\otimes r} = 3^r$. For

$$\boldsymbol{H} = H_{i_1 i_2 \cdots i_r} \boldsymbol{e}_{i_1} \otimes \boldsymbol{e}_{i_2} \otimes \cdots \otimes \boldsymbol{e}_{i_r} \quad \text{and} \quad \boldsymbol{K} = K_{j_1 j_2 \cdots j_r} \boldsymbol{e}_{j_1} \otimes \boldsymbol{e}_{j_2} \otimes \cdots \otimes \boldsymbol{e}_{j_r}, \tag{2.35}$$

we have

$$<\boldsymbol{H}, \boldsymbol{K}> = H_{i_1 i_2 \cdots i_r} K_{i_1 i_2 \cdots i_r}. \tag{2.36}$$

Each orthogonal linear transformation $\boldsymbol{Q}$ on V induces an orthogonal linear transformation $\boldsymbol{Q}^{\otimes r} : V^{\otimes r} \to V^{\otimes r}$ defined by

$$\boldsymbol{Q}^{\otimes r}(\boldsymbol{u}_1 \otimes \cdots \otimes \boldsymbol{u}_r) = \boldsymbol{Q}\boldsymbol{u}_1 \otimes \cdots \otimes \boldsymbol{Q}\boldsymbol{u}_r, \tag{2.37}$$

for all $\boldsymbol{u}_1, \cdots, \boldsymbol{u}_r \in V$.

In continuum physics, many attributes of material points are characterized by multilinear mappings. Let a physical attribute Π of a given material point P be described by an rth-order tensor $\boldsymbol{H}$. When the material point P undergoes a rotation or a rotation followed by an inversion defined by $\boldsymbol{Q} \in \mathrm{O}(3)$, the multilinear mapping that characterizes its attribute Π changes from $\boldsymbol{H}$ to $\mathcal{T}_{\boldsymbol{Q}}\boldsymbol{H}$. We say that Π is characterized by a material tensor $\boldsymbol{H}$ if

$$\mathcal{T}_{\boldsymbol{Q}}\boldsymbol{H} = \boldsymbol{Q}^{\otimes r}\boldsymbol{H}, \tag{2.38}$$

and by a material pseudotensor $\boldsymbol{H}$ if [②]

$$\mathcal{T}_{\boldsymbol{Q}}\boldsymbol{H} = (\det \boldsymbol{Q})\boldsymbol{Q}^{\otimes r}\boldsymbol{H}. \tag{2.39}$$

Particularly, we obtain the effects of inversion on material tensors and pseudotensors as follows. For an rth-order material tensor $\boldsymbol{H}$,

$$\begin{aligned}\mathcal{T}_{\boldsymbol{I}}\boldsymbol{H} = \boldsymbol{I}^{\otimes r}\boldsymbol{H} &= \boldsymbol{I}^{\otimes r}(H_{i_1\cdots i_r}\boldsymbol{e}_{i_1}\otimes\cdots\otimes\boldsymbol{e}_{i_r})\\ &= H_{i_1\cdots i_r}\boldsymbol{I}\boldsymbol{e}_{i_1}\otimes\cdots\otimes\boldsymbol{I}\boldsymbol{e}_{i_r}\\ &= H_{i_1\cdots i_r}(-\boldsymbol{e}_{i_1})\otimes\cdots\otimes(-\boldsymbol{e}_{i_r}) = (-1)^r\boldsymbol{H}.\end{aligned} \tag{2.40}$$

For an rth-order pseudotensor $\boldsymbol{H}$,

$$\begin{aligned}\mathcal{T}_{\boldsymbol{I}}\boldsymbol{H} = (\det\boldsymbol{I})\boldsymbol{I}^{\otimes r}\boldsymbol{H} &= -\boldsymbol{I}^{\otimes r}(H_{i_1\cdots i_r}\boldsymbol{e}_{i_1}\otimes\cdots\otimes\boldsymbol{e}_{i_r})\\ &= -H_{i_1\cdots i_r}\boldsymbol{I}\boldsymbol{e}_{i_1}\otimes\cdots\otimes\boldsymbol{I}\boldsymbol{e}_{i_r}\\ &= -H_{i_1\cdots i_r}(-\boldsymbol{e}_{i_1})\otimes\cdots\otimes(-\boldsymbol{e}_{i_r}) = (-1)^{r+1}\boldsymbol{H}.\end{aligned} \tag{2.41}$$

In continuum mechanics, the stress (**T**) and strain (**E**) inside a solid body are described both by second-order tensors, and are related in a general linear elastic material by a fourth-order elasticity tensor ($\boldsymbol{C}$) and $\mathbf{T} = \boldsymbol{C}[\mathbf{E}]$ [9]. The Levi-Civita symbol $\varepsilon_{ijk} = (\boldsymbol{e}_i \times \boldsymbol{e}_j)\cdot\boldsymbol{e}_k$ is a third order pseudotensor [10]. Here the cross product is taken with respect to the orthonormal basis $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$. And ε_{ijk} can be written as:

$$\varepsilon_{ijk} = \begin{cases} 1, \text{ if } (i,j,k) \text{ is a cyclic (even) permutation of } (1,2,3);\\ -1, \text{ if } (i,j,k) \text{ is a non-cyclic (odd) permutation of } (1,2,3);\\ 0, \text{ otherwise.}\end{cases} \tag{2.42}$$

[②] For brevity, we use $\mathcal{T}_{\boldsymbol{Q}}$ when it acts on both material tensors and pseudotensors with linear transformation $\boldsymbol{Q}$ as in Eqs. (2.38) and in (2.39). Meanwhile this symbol will be also used as the ODF after the linear transformation $\boldsymbol{Q}$ in Chapter 4, in which case it only depends on $\boldsymbol{Q}$, nothing to do with material tensors or pseudotensors. The readers should be beware of the difference in the context.

Particularly, scalars are tensors of zeroth order and vectors are tensors of first order. Mass and volume of a body are scalars. And vectors like velocity, acceleration and force are first-order tensors. Similarly, pseudoscalars are pseudotensors of zeroth order and pseudovectors are pseudotensors of first order. A prime example of pseudovector is the magnetic field. The magnetic flux is the result of the dot product between the surface normal (a vector) and the magnetic field (a pseudovector). Hence the magnetic flux is a pseudoscalar. The gyration tensor, which describes optical activity, is a second-order symmetric pseudotensor. The Righi-Leduc effect, which concerns the effects of a magnetic field on thermal conductivity, is described by a third-order pseudotensor [16].

2.4.2 Complexification of tensor space

Let $V_c = \{\boldsymbol{u} + \sqrt{-1}\boldsymbol{v} : \boldsymbol{u} \in V, \boldsymbol{v} \in V\}$ be the complexification of V [19, 34]. We equip V_c with the Hermitian product induced by the inner product in V for real vectors. The Hermitian product of two vectors $\boldsymbol{w} = (w_1, w_2, w_3)$ and $\boldsymbol{z} = (z_1, z_2, z_3)$ in V_c is given by $<\boldsymbol{w}, \boldsymbol{z}> = w_i \overline{z_i}$ for $i = 1, 2, 3$. Each orthogonal linear transformation $\boldsymbol{Q}$ on V has a natural extension to a linear transformation on V_c, which we still denote by $\boldsymbol{Q}$, defined as follows:

$$\boldsymbol{Q}(\boldsymbol{u} + \sqrt{-1}\boldsymbol{v}) = \boldsymbol{Q}\boldsymbol{u} + \sqrt{-1}\boldsymbol{Q}\boldsymbol{v} \tag{2.43}$$

for each $\boldsymbol{u}$, $\boldsymbol{v}$ in V. As each transformation $\boldsymbol{Q} : V \to V$ is orthogonal, its extension $\boldsymbol{Q} : V_c \to V_c$ is unitary.

Let $V_c^{\otimes r}$ be the complexification of $V^{\otimes r}$. It is clear that $V_c^{\otimes r} = V_c \otimes V_c \otimes \cdots \otimes V_c$ (r factors). We equip $V_c^{\otimes r}$ with the Hermitian product satisfying (2.34) for all $\boldsymbol{u}_1, \cdots, \boldsymbol{u}_r$ and $\boldsymbol{v}_1, \cdots, \boldsymbol{v}_r$ in V_c, which is induced by the Hermitian product on V_c. Under this Hermitian product, for two rth-order tensors $\boldsymbol{H}, \boldsymbol{K}$ as in (2.35), we obtain the following formula as an extension of (2.36):

$$<\boldsymbol{H}, \boldsymbol{K}> = H_{i_1 i_2 \cdots i_r} \overline{K_{i_1 i_2 \cdots i_r}}. \tag{2.44}$$

Similarly each operator $\boldsymbol{Q} \in \mathrm{O}(3)$ on V_c induces a linear transformation $\boldsymbol{Q}^{\otimes r}$ on $V_c^{\otimes r}$ defined by (2.37) for all $\boldsymbol{u}_1, \cdots, \boldsymbol{u}_r$ in V_c.

The mappings $\Phi_r : \mathrm{O}(3) \to \mathrm{GL}(V_c^{\otimes r})$, $\boldsymbol{Q} \mapsto \boldsymbol{Q}^{\otimes r}$ (cf. (2.38) for material tensors) and $\Phi_p : \mathrm{O}(3) \to \mathrm{GL}(V_c^{\otimes r})$, $\boldsymbol{Q} \mapsto (\det \boldsymbol{Q})\boldsymbol{Q}^{\otimes r}$ (cf. (2.39) for material pseudotensors) are representations of O(3) on $V_c^{\otimes r}$. To see this, it is sufficient to show that Φ_p is indeed a representaion of O(3) (the proof for Φ_r is similar but simpler). Let $\boldsymbol{E}$ be the identity in O(3), clearly $(\det \boldsymbol{E})\boldsymbol{E}^{\otimes r} = \boldsymbol{E}^{\otimes r}$ is an identity operator on $V_c^{\otimes r}$ by (2.37). And for $\boldsymbol{Q}_1, \boldsymbol{Q}_2 \in \mathrm{O}(3)$, $\det(\boldsymbol{Q}_1\boldsymbol{Q}_2)(\boldsymbol{Q}_1\boldsymbol{Q}_2)^{\otimes r} = (\det \boldsymbol{Q}_1)(\det \boldsymbol{Q}_2)\boldsymbol{Q}_1^{\otimes r}\boldsymbol{Q}_2^{\otimes r} = (\det \boldsymbol{Q}_1)\boldsymbol{Q}_1^{\otimes r}(\det \boldsymbol{Q}_2)\boldsymbol{Q}_2^{\otimes r}$. Hence by Definition (2.3.1) Φ_p is a representation of O(3).

Moreover, the representations Φ_r and Φ_p are unitary and continuous. Indeed, by Eqs. (2.31) and (2.37), since $\boldsymbol{Q} : V_c \to V_c$ is unitary, both $\boldsymbol{Q}^{\otimes r}$ and $(\det \boldsymbol{Q})\boldsymbol{Q}^{\otimes r} : V_c^{\otimes r} \to V_c^{\otimes r}$ are unitary. As for continuity of the representations Φ_r and Φ_p, note that the matrix elements of $\boldsymbol{Q}^{\otimes r}$ and $(\det \boldsymbol{Q})\boldsymbol{Q}^{\otimes r}$ under the basis $\{\boldsymbol{e}_{i_1} \otimes \boldsymbol{e}_{i_2} \otimes \cdots \otimes \boldsymbol{e}_{i_r} : 1 \leq i_k \leq 3 \text{ for } k = 1, \cdots r\}$ are polynomial functions of Q_{ij}, the matrix elements of $\boldsymbol{Q}$ under the basis $\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3$.

Chapter 3 Decomposition formulas for tensors and pseudotensors under O(3)

3.1 A complete set of irreducible representations of O(3)

We have introduced some basic concepts of group representations and the irreducible representations of SO(3). In this section, we will present the irreducible representations of O(3).

The irreducible representations of the orthogonal group O(3), which is compact, can be obtained from those of SO(3). The rotation group SO(3) is a normal subgroup of index two in O(3). The left coset decomposition of O(3) is $\mathrm{O}(3) = \{\mathrm{SO}(3), \boldsymbol{I}\mathrm{SO}(3)\}$, where $\boldsymbol{I}$ is the inversion.

Theorem 3.1.1. *A complete set of irreducible unitary representations of O(3) is given by* $\mathcal{D}_l^{\pm}$ *of dimension* $2l+1$ *(*$l = 0, 1, 2, \cdots$*), which are defined by* $\mathcal{D}_l^{\pm} : \boldsymbol{Q} \mapsto [D_{mn}^{l,\pm}(\boldsymbol{Q})]$ *(*$-l \leq m \leq l, -l \leq n \leq l$*), where* $\boldsymbol{Q} \in \mathrm{O}(3)$*, and*

$$D_{mn}^{l,+}(\boldsymbol{Q}) = \begin{cases} D_{mn}^{l}(\boldsymbol{R}), \text{ if } \boldsymbol{Q} = \boldsymbol{R} \in \mathrm{SO}(3); \\ D_{mn}^{l}(\boldsymbol{R}), \text{ if } \boldsymbol{Q} = \boldsymbol{IR} \in \boldsymbol{I}\mathrm{SO}(3). \end{cases} \tag{3.1}$$

$$D_{mn}^{l,-}(\boldsymbol{Q}) = \begin{cases} D_{mn}^{l}(\boldsymbol{R}), \text{ if } \boldsymbol{Q} = \boldsymbol{R} \in \mathrm{SO}(3); \\ -D_{mn}^{l}(\boldsymbol{R}), \text{ if } \boldsymbol{Q} = \boldsymbol{IR} \in \boldsymbol{I}\mathrm{SO}(3). \end{cases} \tag{3.2}$$

We shall need the following lemma for our proof of the theorem.

Lemma 3.1.2. *Let* Z_c *be a finite-dimensional complex vector space. Let* $\widetilde{\mathcal{D}} : \mathrm{O}(3) \to \mathrm{GL}(Z_c)$ *be an irreducible unitary representation of* O(3) *on* Z_c*. Then* $\widetilde{\mathcal{D}}(\boldsymbol{I}) = \lambda \boldsymbol{E}$ *for some* $\lambda \in \mathbb{C}$*; here* $\boldsymbol{E}$ *is the identity operator in* Z_c*.*

Proof of Lemma 3.1.2. By the fundamental theorem of algebra $\widetilde{\mathcal{D}}(\boldsymbol{I})$, as a linear operator, has at least one eigenvalue. Let λ be an eigenvalue of $\widetilde{\mathcal{D}}(\boldsymbol{I})$, and let $Z_1 = \{x \in Z_c : \widetilde{\mathcal{D}}(\boldsymbol{I})x = \lambda x\}$. Since λ is an eigenvalue, Z_1 is not empty. Choose $x \in Z_1$; then $\widetilde{\mathcal{D}}(\boldsymbol{I})x = \lambda x$. Let $\boldsymbol{Q} \in$ O(3). Since $\boldsymbol{I}$ commutes with all elements of O(3), we have $\widetilde{\mathcal{D}}(\boldsymbol{I})\widetilde{\mathcal{D}}(\boldsymbol{Q})x = \widetilde{\mathcal{D}}(\boldsymbol{Q})\widetilde{\mathcal{D}}(\boldsymbol{I})x = \widetilde{\mathcal{D}}(\boldsymbol{Q})\lambda x = \lambda\widetilde{\mathcal{D}}(\boldsymbol{Q})x$ for any $\boldsymbol{Q} \in$ O(3). Thus $\widetilde{\mathcal{D}}(\boldsymbol{Q})x \in Z_1$ for any $\boldsymbol{Q} \in$ O(3). Since $\widetilde{\mathcal{D}}$ is irreducible, we conclude that $Z_1 = Z_c$. Thus we have $\widetilde{\mathcal{D}}(\boldsymbol{I})x = \lambda x$ for all $x \in Z_c$, and this completes the proof. □

Proof of Theorem 3.1.1. [1, 24] Let $\widetilde{\mathcal{D}}$ be a finite-dimensional irreducible unitary representation of O(3). By Lemma 3.1.2 and the fact that $\widetilde{\mathcal{D}}(\boldsymbol{I})^2 = \widetilde{\mathcal{D}}(\boldsymbol{I}^2) = \widetilde{\mathcal{D}}(\boldsymbol{E}) = \boldsymbol{E}$, we have $\widetilde{\mathcal{D}}(\boldsymbol{I}) = \pm\boldsymbol{E}$. It follows that $\widetilde{\mathcal{D}}|$SO(3) is still irreducible. Indeed, if it is reducible in space Z_c and has $Z' \subset Z_c$ as a non-zero proper subspace on which $\widetilde{\mathcal{D}}|$SO(3) is invariant, then $\widetilde{\mathcal{D}}|$O(3) is irreducible in Z' and thus $\widetilde{\mathcal{D}}|$O(3) is reducible in Z_c, which contradicts the assumption. Therefore $\widetilde{\mathcal{D}}|\mathrm{SO}(3) \cong \mathcal{D}_l$ for some $l = 0, 1, 2, \cdots$. With the fact $\widetilde{\mathcal{D}}(\boldsymbol{I}) = \pm\boldsymbol{E}$, we have $\widetilde{\mathcal{D}}(\boldsymbol{R}) = \mathcal{D}_l(\boldsymbol{R})$ and $\widetilde{\mathcal{D}}(\boldsymbol{IR}) = \pm\mathcal{D}_l(\boldsymbol{R})$ for any $\boldsymbol{R} \in$ SO(3). It follows that for each $l = 0, 1, 2, ...$, there are two irreducible representations of O(3), namely $\mathcal{D}_l^+$, $\mathcal{D}_l^-$ which are defined by (3.1) and (3.2).

The representations $\mathcal{D}_l^\pm$ are not only irreducible, but they are also pairwise-inequivalent, continuous and unitary, which can be easily seen by the relations between $\mathcal{D}_l^\pm$ and $\mathcal{D}_l$ and the fact that $\mathcal{D}_l$ has these properties.

Furthermore, the family of $\{\mathcal{D}_l^\pm\}$ is a complete set of irreducible representations of the orthogonal group (O(3)). To show this, we need to show every irreducible representation of O(3) is equivalent to one of the representations $\mathcal{D}_l^\pm$ which are irreducible and pairwise inequivalent. Indeed, let T be an irreducible unitary representation of O(3). Then $T|$SO(3) has to be equivalent to one of $\mathcal{D}_l$ by the fact that the family $\{\mathcal{D}_l\}$ is a complete set of irreducible unitary representations of SO(3). Without loss of generality, say $T|$SO(3) is equivalent to $\mathcal{D}_k$. Because $T(\boldsymbol{I}) = \pm\boldsymbol{E}$ (Lemma 3.1.2), T is equivalent to $\mathcal{D}_k^+$ or $\mathcal{D}_k^-$. □

Remark: We can also obtain expressions of the two families $\mathcal{D}_l^+$, $\mathcal{D}_l^-$ of irreducible representations of O(3) by a general theorem as follows. Let $\{T_{G_1}^i\}$ and $\{T_{G_2}^\mu\}$ be complete sets of irreducible unitary representations of finite or compact groups G_1 and G_2, respectively. Then a complete set of irreducible unitary representations of the direct product $G_1 \times G_2$ is given by the family $\{T_{G_1}^i \otimes T_{G_2}^\mu\}$ of tensor products of representations in $\{T_{G_1}^i\}$ and $\{T_{G_2}^\mu\}$ [15].

The table of irreducible representations for $C_i = \{\boldsymbol{E}, \boldsymbol{I}\}$ is given as follows [37]:

C_i	e	i
D^1	1	1
D^2	1	−1

(3.3)

Since O(3) can be written as the direct product of C_i and SO(3) (i.e. O(3) = C_i×SO(3)), the matrix elements of the irreducible representations of O(3) are given by products as follows:

$\boldsymbol{Q} \in$ O(3)	$\boldsymbol{Q} = \boldsymbol{R} \in$ SO(3)	$\boldsymbol{Q} = \boldsymbol{IR} \in \boldsymbol{I}$SO(3)
$D_{mn}^{l,+}(\boldsymbol{Q})$	$1 \times D_{mn}^l(\boldsymbol{R})$	$1 \times D_{mn}^l(\boldsymbol{R})$
$D_{mn}^{l,-}(\boldsymbol{Q})$	$1 \times D_{mn}^l(\boldsymbol{R})$	$-1 \times D_{mn}^l(\boldsymbol{R})$

(3.4)

Of course, (3.4) agrees with (3.1) and (3.2).

3.2 Characters of the irreducible representations of O(3)

Let $\chi_l^\pm(\boldsymbol{Q}) = \mathrm{tr}[D_{mn}^{l,\pm}(\boldsymbol{Q})]$ and $\chi_l(\boldsymbol{R}) = \mathrm{tr}[D_{mn}^l(\boldsymbol{R})]$ be the characters of the representations $\mathcal{D}_l^\pm$ of O(3) and $\mathcal{D}_l$ of SO(3), respectively. Since elements in the orthogonal group can be considered as rotations or rotations followed by inversions, by Theorem 3.1.1 we have

$$\chi_l^\pm(\boldsymbol{R}(\boldsymbol{n}, \omega)) = \mathrm{tr}[D_{mn}^{l,\pm}(\boldsymbol{R}(\boldsymbol{n}, \omega))] = \mathrm{tr}[D_{mn}^l(\boldsymbol{R}(\boldsymbol{n}, \omega))] = \chi_l(\boldsymbol{R}(\boldsymbol{n}, \omega)) \tag{3.5}$$

$$
\begin{aligned}
\chi_l^+(\boldsymbol{IR}(\boldsymbol{n},\omega)) &= \mathrm{tr}[D^{l,+}_{mn}(\boldsymbol{IR}(\boldsymbol{n},\omega))] = \mathrm{tr}[D^{l}_{mn}(\boldsymbol{R}(\boldsymbol{n},\omega))] = \chi_l(\boldsymbol{R}(\boldsymbol{n},\omega)) \\
&= -\mathrm{tr}[D^{l,-}_{mn}(\boldsymbol{IR}(\boldsymbol{n},\omega))] = -\chi_l^-(\boldsymbol{IR}(\boldsymbol{n},\omega))
\end{aligned}
\tag{3.6}
$$

where [20],

$$
\chi_l(\boldsymbol{R}(\boldsymbol{n},\omega)) = 1 + 2\sum_{k=0}^{l}\cos k\omega = \begin{cases} \dfrac{\sin(l+\frac{1}{2})\omega}{\sin\frac{1}{2}\omega} & \text{for } \omega \neq 0 \\ 2l+1 & \text{for } \omega = 0 \end{cases}
\tag{3.7}
$$

In summary,

$$
\chi_l^{\pm}(\boldsymbol{R}(\boldsymbol{n},\omega)) = \chi_l(\boldsymbol{R}(\boldsymbol{n},\omega))
\tag{3.8}
$$

$$
\chi_l^+(\boldsymbol{IR}(\boldsymbol{n},\omega)) = -\chi_l^-(\boldsymbol{IR}(\boldsymbol{n},\omega)) = \chi_l(\boldsymbol{R}(\boldsymbol{n},\omega))
\tag{3.9}
$$

By direct computation, we find that

$$
\begin{aligned}
\int_{\mathrm{O(3)}} |\chi_l^+|^2 dg &= \int_{\mathrm{O(3)}} |\chi_l^-|^2 dg = 2\int_{\mathrm{SO(3)}} |\chi_l|^2 dg \\
&= 2\cdot\frac{1}{16\pi^2}\int_{\mathrm{SO(3)}} |\chi_l|^2 dV = 2\cdot\frac{1}{16\pi^2}\int_{\mathrm{SO(3)}} |\chi_l|^2 \sin\theta d\psi d\theta d\phi \\
&= 2\cdot\frac{1}{16\pi^2}\int_{\mathrm{SO(3)}} |\chi_l|^2 4\sin^2\frac{\omega}{2} sin\Theta d\omega d\Theta d\Phi \\
&= 2\cdot\frac{1}{16\pi^2}\int_0^{2\pi}\int_0^{\pi} 4 sin\Theta d\Theta d\Phi \int_0^{\pi} |\chi_l|^2 \sin^2\frac{\omega}{2} d\omega \\
&= 2\cdot\frac{16\pi}{16\pi^2}\int_0^{\pi} |\chi_l(\omega)|^2 \sin^2\frac{\omega}{2} d\omega \\
&= \frac{2}{\pi}\int_0^{\pi} |\chi_l(\omega)|^2 \sin^2\frac{\omega}{2} d\omega \\
&= 1,
\end{aligned}
\tag{3.10}
$$

where we have appealed to the axis-angle $(\boldsymbol{n}(\Theta,\Phi),\omega)$ parametrization of rotations (cf. (2.25)).

This also shows that the representation $\mathcal{D}_l^{\pm}$ is irreducible.

Remark: As we have discussed earlier, the orthogonal group O(3) can be taken as the disjoint union of SO(3) and $\boldsymbol{I}$SO(3), each of which has a natural Riemannian-manifold structure. Pertaining to the Riemannian metric the orthogonal group has a bi-invariant volume measure (thus also a Haar measure) $\mathcal{V}$, which is related to the normalized Haar measure g by the formula $\mathcal{V} = 16\pi^2 g$. Here we use the measure g instead of $\mathcal{V}$ to conform to standard practice in the theory of group representations, i.e., let the compact group in question have unit group volume.

The family of pairwise-inequivalent, continuous, irreducible unitary representations $\mathcal{D}_l^{\pm}$ $(l = 0, 1, 2, \cdots)$ is complete, i.e., any irreducible unitary representation of the orthogonal group is equivalent to one of the $\mathcal{D}_l^{\pm}$'s. In particular, let $\boldsymbol{Q} \mapsto \boldsymbol{Q}^{\otimes r}|Z_c$ be an irreducible unitary representation of the orthogonal group on Z_c which is equivalent to $\mathcal{D}_k^{+}$ or $\mathcal{D}_k^{-}$. There exists then a basis $\boldsymbol{A}_m$ $(-k \leq m \leq k)$ in Z_c such that

$$\boldsymbol{Q}^{\otimes r}\boldsymbol{A}_m = \sum_{p=-k}^{k} D_{pm}^{k,\pm}(\boldsymbol{Q})\boldsymbol{A}_p. \tag{3.11}$$

By taking complex-conjugate on both sides of the preceding equation, we see that there also exists a basis $\boldsymbol{B}_m = \overline{\boldsymbol{A}_m}$ $(-k \leq m \leq k)$ in Z_c such that

$$\boldsymbol{Q}^{\otimes r}\boldsymbol{B}_m = \sum_{p=-k}^{k} \overline{D_{pm}^{k,\pm}(\boldsymbol{Q})}\boldsymbol{B}_p = \sum_{p=-k}^{k} D_{mp}^{k,\pm}(\boldsymbol{Q}^T)\boldsymbol{B}_p, \tag{3.12}$$

where we have appealed to Eq. (2.29). The mapping $\boldsymbol{Q} \mapsto [\overline{D_{mn}^{l,\pm}(\boldsymbol{Q})}]$ is none other than the contragradient representation of $\mathcal{D}_l^{\pm}$; hence it is also irreducible. We say that the tensors $\boldsymbol{B}_m$ $(-k \leq m \leq k)$ constitute an irreducible tensor basis (with respect to the orthogonal group O(3)), because they form the basis for an irreducible representation of O(3).

Let $L^2(\mathrm{O}(3))$ be the Hilbert space of complex-valued square-integrable functions defined on the orthogonal group. Note that all $D_{pm}^{l,\pm}$ functions belong to $L^2(\mathrm{O}(3))$. The inner product $<\cdot,\cdot>$ on $L^2(\mathrm{O}(3))$ is defined by

$$<f, g> = \int_{\mathrm{O}(3)} f(\boldsymbol{R})\overline{g(\boldsymbol{R})}dg \tag{3.13}$$

for all f, g in $L^2(\mathrm{O}(3))$. Since the orthogonal group is compact, it follows from the theory of group representations that the functions $D^{l,\pm}_{mn}(\cdot)$, being the matrix elements of a complete set of mutually-inequivalent, irreducible, continuous unitary representations of the orthogonal group, satisfy the orthogonality relation

$$< D^{l,+}_{mn}, D^{l',+}_{m'n'} > = \int_{\mathrm{O}(3)} D^{l,+}_{mn}(\boldsymbol{Q})\overline{D^{l',+}_{m'n'}(\boldsymbol{Q})}dg = \frac{1}{2l+1}\delta_{ll'}\delta_{mm'}\delta_{nn'}, \tag{3.14}$$

$$< D^{l,-}_{mn}, D^{l',-}_{m'n'} > = \int_{\mathrm{O}(3)} D^{l,-}_{mn}(\boldsymbol{Q})\overline{D^{l',-}_{m'n'}(\boldsymbol{Q})}dg = \frac{1}{2l+1}\delta_{ll'}\delta_{mm'}\delta_{nn'}, \tag{3.15}$$

where the Kronecker delta (δ_{ij}) is defined as

$$\delta_{ij} = \begin{cases} 1, \text{ if } i = j; \\ 0, \text{ if } i \neq j. \end{cases} \tag{3.16}$$

and

$$< D^{l,+}_{mn}, D^{l',-}_{m'n'} > = < D^{l,-}_{mn}, D^{l',+}_{m'n'} > = 0, \tag{3.17}$$

and they constitute an orthogonal basis in $L^2(\mathrm{O}(3))$. From the orthogonality relations of the matrix elements follow the orthogonality relations of the characters (denoted by $\chi^{\pm}_l$), namely:

$$\begin{aligned} <\chi^+_l, \chi^+_{l'}> &= \sum_{m=-l}^{l}\sum_{m'=-l'}^{l'} \int_{\mathrm{O}(3)} D^{l,+}_{mm}(\boldsymbol{Q})\overline{D^{l',+}_{m'm'}(\boldsymbol{Q})}dg \\ &= \sum_{m=-l}^{l}\sum_{m'=-l'}^{l'} \frac{\delta_{ll'}\delta_{mm'}}{2l+1} = \sum_{m=-l}^{l} \frac{\delta_{ll'}}{2l+1} = \delta_{ll'}. \end{aligned} \tag{3.18}$$

and

$$<\chi^-_l, \chi^-_{l'}> = \delta_{ll'}, \qquad <\chi^+_l, \chi^-_{l'}> = <\chi^-_l, \chi^+_{l'}> = 0. \tag{3.19}$$

As illustration, we give a proof that $<\chi_l^+, \chi_{l'}^-> = 0$:

$$
\begin{aligned}
<\chi_l^+, \chi_{l'}^-> &= \sum_{m=-l}^{l} \sum_{m'=-l'}^{l'} \int_{\mathrm{O}(3)} D_{mm}^{l,+}(\boldsymbol{Q}) \overline{D_{m'm'}^{l',-}(\boldsymbol{Q})} dg \\
&= \sum_{m=-l}^{l} \sum_{m'=-l'}^{l'} \int_{\mathrm{SO}(3)} D_{mm}^{l,+}(\boldsymbol{R}) \overline{D_{m'm'}^{l',-}(\boldsymbol{R})} dg \\
&\quad + \sum_{m=-l}^{l} \sum_{m'=-l'}^{l'} \int_{\boldsymbol{I}\mathrm{SO}(3)} D_{mm}^{l,+}(\boldsymbol{IR}) \overline{D_{m'm'}^{l',-}(\boldsymbol{IR})} dg \\
&= \sum_{m=-l}^{l} \sum_{m'=-l'}^{l'} \int_{\mathrm{SO}(3)} D_{mm}^{l}(\boldsymbol{R}) \overline{D_{m'm'}^{l'}(\boldsymbol{R})} dg \\
&\quad + \sum_{m=-l}^{l} \sum_{m'=-l'}^{l'} \int_{\mathrm{SO}(3)} D_{mm}^{l}(\boldsymbol{R}) (-\overline{D_{m'm'}^{l'}(\boldsymbol{R})}) dg \\
&= 0.
\end{aligned}
\tag{3.20}
$$

3.3 Decomposition of a tensor or pseudotensor into its irreducible parts under O(3)

A subspace $Z \subset V^{\otimes r}$ (See Sec 2.4) is said to be invariant under the action of the orthogonal group (O(3)) if it remains invariant under $\boldsymbol{Q}^{\otimes r}$ for each operator $\boldsymbol{Q} \in \mathrm{O}(3)$. If Z is an invariant subspace of $V^{\otimes r}$ under the action of the orthogonal group, then its complexification Z_c is an invariant subspace of $V_c^{\otimes r}$. Since every finite-dimensional continuous unitary representation of a compact group is completely reducible, each tensor representation of the orthogonal group $\rho : \boldsymbol{Q} \mapsto \boldsymbol{Q}^{\otimes r}|Z_c$ can be decomposed as a direct sum of irreducible subrepresentations, each of which is equivalent to some $\mathcal{D}_k^{\pm}$ $(k := 1, 2, \cdots, r)$:

$$
Z_c = m_0^+ \mathcal{D}_0^+ + m_1^+ \mathcal{D}_1^+ + \cdots + m_r^+ \mathcal{D}_r^+ + m_0^- \mathcal{D}_0^- + m_1^- \mathcal{D}_1^- + \cdots + m_r^- \mathcal{D}_r^-, \tag{3.21}
$$

where m_k is the multiplicity of $\mathcal{D}_k^{\pm}$ in the decomposition.

Let χ_ρ be the character of the representation $\rho : \boldsymbol{Q} \mapsto \boldsymbol{Q}^{\otimes r}|Z_c$ with $\boldsymbol{Q} \in \mathrm{O}(3)$, which decomposes into the direct sum given in Eq. (3.21). This decomposition dictates that we have

$$
\chi_\rho = m_0^+ \chi_0^+ + m_1^+ \chi_1^+ + \cdots + m_r^+ \chi_r^+ + m_0^- \chi_0^- + m_1^- \chi_1^- + \cdots + m_r^- \chi_r^-. \tag{3.22}
$$

By Eqs. (3.18) and (3.22) we obtain the following formula for the multiplicities $m_k^\pm$ ($k = 0, 1, ..., r$) in the decomposition (3.21); for brevity, we shall write $\chi(\omega) = \chi(\boldsymbol{R}(\boldsymbol{n}, \omega))$ and $\chi(\boldsymbol{I}, \omega) = \chi(\boldsymbol{I}\boldsymbol{R}(\boldsymbol{n}, \omega))$:

$$
\begin{aligned}
m_k^\pm = \; &<\chi_\rho, \chi_k^\pm> = \int_{\mathrm{O}(3)} \chi_\rho \overline{\chi_k^\pm} dg = \int_{\mathrm{SO}(3)} \chi_\rho \overline{\chi_k^\pm} dg + \int_{\boldsymbol{I}\mathrm{SO}(3)} \chi_\rho \overline{\chi_k^\pm} dg \\
=&\frac{1}{16\pi^2} \int_0^{2\pi} \int_0^{\pi} \int_0^{\pi} 4\chi_\rho(\omega)\overline{\chi_k^\pm(\omega)} \sin^2 \frac{\omega}{2} \sin\Theta d\Theta d\Phi d\omega \\
+&\frac{1}{16\pi^2} \int_0^{2\pi} \int_0^{\pi} \int_0^{\pi} 4\chi_\rho(\boldsymbol{I}, \omega)\overline{\chi_k^\pm(\boldsymbol{I}, \omega)} \sin^2 \frac{\omega}{2} \sin\Theta d\Theta d\Phi d\omega \\
=&\frac{1}{16\pi^2} \int_0^{\pi} (\int_0^{2\pi} \int_0^{\pi} 4 \sin\Theta d\Theta d\Phi)\chi_\rho(\omega)\overline{\chi_k^\pm(\omega)} \sin^2 \frac{\omega}{2} d\omega \\
+&\frac{1}{16\pi^2} \int_0^{\pi} (\int_0^{2\pi} \int_0^{\pi} 4 \sin\Theta d\Theta d\Phi)\chi_\rho(\boldsymbol{I}, \omega)\overline{\chi_k^\pm(\boldsymbol{I}, \omega)} \sin^2 \frac{\omega}{2} d\omega \\
=&\frac{16\pi}{16\pi^2} \int_0^{\pi} \chi_\rho(\omega)\overline{\chi_k^\pm(\omega)} \sin^2 \frac{\omega}{2} d\omega + \frac{16\pi}{16\pi^2} \int_0^{\pi} \chi_\rho(\boldsymbol{I}, \omega)\overline{\chi_k^\pm(\boldsymbol{I}, \omega)} \sin^2 \frac{\omega}{2} d\omega \\
=&\frac{1}{\pi} \int_0^{\pi} \chi_\rho(\omega)\overline{\chi_k^\pm(\omega)} \sin^2 \frac{\omega}{2} d\omega + \frac{1}{\pi} \int_0^{\pi} \chi_\rho(\boldsymbol{I}, \omega)\overline{\chi_k^\pm(\boldsymbol{I}, \omega)} \sin^2 \frac{\omega}{2} d\omega,
\end{aligned}
\tag{3.23}
$$

where the fourth equality is obtained by using axis-angle parameters ([18, 40]; see also (2.25)) and $\overline{\chi_k^\pm}$ denotes the complex conjugate of $\chi_k^\pm$; here $\overline{\chi_k^\pm} = \chi_k^\pm$ because $\chi_k^\pm$ is real.

Hence, once the character χ_ρ of a representation $\rho : \boldsymbol{Q} \mapsto \boldsymbol{Q}^{\otimes r}|Z_c$ is obtained, the decomposition formula for the representation follows immediately (see some examples in [20, 42], particularly on rotational groups).

In this work we will specify more about the decomposition formula (3.21) for tensor representations and its counterpart for pseudotensor representations of the orthogonal group through the following lemma and theorem.

Lemma 3.3.1. *For $k \geq 1$, let Z be a $(2k+1)$-dimensional subspace of the tensor space $V^{\otimes r}$ invariant under $\boldsymbol{R}^{\otimes r}$ for each $\boldsymbol{R} \in \mathrm{SO}(3)$, and let Z_c be its complexification. Suppose the representation $\boldsymbol{R} \mapsto \boldsymbol{R}^{\otimes r}|Z_c$ is equivalent to the irreducible unitary representation $\mathcal{D}_k$. Then Z_c is invariant under $\mathcal{T}_{\boldsymbol{Q}} : V_c^{\otimes r} \to V_c^{\otimes r}$ for each $\boldsymbol{Q} \in \mathrm{O}(3)$, where $\mathcal{T}_{\boldsymbol{Q}} = \boldsymbol{Q}^{\otimes r}$ for material tensors and $\mathcal{T}_{\boldsymbol{Q}} = (\det \boldsymbol{Q})\boldsymbol{Q}^{\otimes r}$ for material pseudotensors, respectively. For material* *tensors, the representation* $\boldsymbol{Q} \mapsto \mathcal{T}_{\boldsymbol{Q}}|Z_c$ *is equivalent to* $\mathcal{D}_k^+$ *if* r *is even and to* $\mathcal{D}_k^-$ *if* r *is odd. For material pseudotensors, the representation* $\boldsymbol{Q} \mapsto \mathcal{T}_{\boldsymbol{Q}}|Z_c$ *is equivalent to* $\mathcal{D}_k^+$ *if* r *is odd and to* $\mathcal{D}_k^-$ *if* r *is even.*

Proof. Under both transformation laws (2.38) and (2.39), we have $\mathcal{T}_{\boldsymbol{I}}\boldsymbol{H} = \pm\boldsymbol{H}$ for any $\boldsymbol{H} \in Z_c$; cf. (2.40) and (2.41). Since Z_c is invariant under $\boldsymbol{R}^{\otimes r}$, it is also invariant under $(\boldsymbol{IR})^{\otimes r} = \boldsymbol{I}^{\otimes r}\boldsymbol{R}^{\otimes r}$ and $(\det(\boldsymbol{IR}))(\boldsymbol{IR})^{\otimes r} = -\boldsymbol{I}^{\otimes r}\boldsymbol{R}^{\otimes r}$. It follows that Z_c is invariant under $\mathcal{T}_{\boldsymbol{Q}}$ for each $\boldsymbol{Q} \in \mathrm{O}(3)$.

Consider first the case of material tensors, which obey the transformation law $\mathcal{T}_{\boldsymbol{Q}} = \boldsymbol{Q}^{\otimes r}$. Let $\rho : \mathrm{O}(3) \to \mathrm{GL}(Z_c)$ be the representation $\boldsymbol{Q} \mapsto \boldsymbol{Q}^{\otimes r}|Z_c$. By the hypothesis that the representation $\boldsymbol{R} \mapsto \boldsymbol{R}^{\otimes r}|Z_c$ is equivalent to the irreducible unitary representation $\mathcal{D}_k$ of SO(3), there exists an orthonormal basis $\boldsymbol{H}_m$ [①] $(-k \le m \le k)$ such that

$$\boldsymbol{R}^{\otimes r}\boldsymbol{H}_m = \sum_{p=-k}^{k} D_{mp}^k(\boldsymbol{R}^T)\boldsymbol{H}_p \qquad \text{for each } \boldsymbol{R} \in \mathrm{SO}(3). \tag{3.24}$$

It follows from (2.40) and (3.24) that

$$\begin{aligned}(\boldsymbol{IR})^{\otimes r}\boldsymbol{H}_m &= \boldsymbol{I}^{\otimes r}\left(\boldsymbol{R}^{\otimes r}\boldsymbol{H}_m\right)\\ &= (-1)^r \sum_{p=-k}^{k} D_{mp}^k(\boldsymbol{R}^T)\boldsymbol{H}_p \qquad \text{for each } \boldsymbol{R} \in \mathrm{SO}(3).\end{aligned} \tag{3.25}$$

We obtain from (3.24) and (3.25) that

$$\begin{aligned}\chi_\rho(\boldsymbol{Q}) &= \begin{cases}\chi_k(\boldsymbol{R}) & \text{for } \boldsymbol{Q} = \boldsymbol{R}\\ (-1)^r\chi_k(\boldsymbol{R}) & \text{for } \boldsymbol{Q} = \boldsymbol{IR}\end{cases}\\ &= \begin{cases}\chi_k^+(\boldsymbol{Q}) & \text{if } r \text{ is even}\\ \chi_k^-(\boldsymbol{Q}) & \text{if } r \text{ is odd.}\end{cases}\end{aligned} \tag{3.26}$$

[①] Man and Huang [20] showed the existence of an orthonormal set of irreducible basis tensors $\boldsymbol{H}_m^{k,s}$ $(-k \le m \le k,\ 1 \le s \le n_k$ where n_k is the multiplicity of $\mathcal{D}_k)$ which together span Z_c, and they developed a procedure to determine explicitly $\boldsymbol{H}_m^{k,s}$.

Hence we conclude that for material tensors the representation $\boldsymbol{Q} \mapsto \mathcal{T}_{\boldsymbol{Q}}|Z_c$ is equivalent to $\mathcal{D}_k^+$ if r is even and to $\mathcal{D}_k^-$ if r is odd.

For pseudotensors, which observe the transformation law $\mathcal{T}_{\boldsymbol{Q}} = (\det \boldsymbol{Q})\boldsymbol{Q}^{\otimes r}$, instead of (3.25) we derive from (2.41) the formula that

$$(\det(\boldsymbol{IR}))(\boldsymbol{IR})^{\otimes r}\boldsymbol{H}_m = (-1)^{r+1}\sum_{p=-k}^{k} D^k_{mp}(\boldsymbol{R}^T)\boldsymbol{H}_p \qquad \text{for each } \boldsymbol{R} \in \mathrm{SO}(3), \tag{3.27}$$

from which it follows that the representation $\mathcal{T}_{\boldsymbol{Q}}|Z_c$ is equivalent to $\mathcal{D}_k^+$ if r is odd and to $\mathcal{D}_k^-$ if r is even. □

Corollary 3.3.2. *The representation* $\boldsymbol{Q} \mapsto \mathcal{T}_{\boldsymbol{Q}}|Z_c$ *described in* Lemma 3.3.1 *satisfy the condition: For each* $\boldsymbol{Q} \in \mathrm{O}(3)$*,*

$$\mathcal{T}_{\boldsymbol{Q}}\boldsymbol{H}_m = \begin{cases} \sum_{p=-k}^{k} D^{k,+}_{mp}(\boldsymbol{Q}^T)\boldsymbol{H}_p, & \textit{for even order } [\mathrm{r}] \textit{ and odd order } [\mathrm{p}]; \\ \sum_{p=-k}^{k} D^{k,-}_{mp}(\boldsymbol{Q}^T)\boldsymbol{H}_p, & \textit{for odd order } [\mathrm{r}] \textit{ and even order } [\mathrm{p}]. \end{cases} \tag{3.28}$$

Here [r] *denotes material tensors (regular) and* [p] *denotes pseudotensors.*

Proof. For material tensors, we have from (3.1), (3.2) and (3.24) that

$$\mathcal{T}_{\boldsymbol{Q}}\boldsymbol{H}_m = \boldsymbol{Q}^{\otimes r}\boldsymbol{H}_m = \sum_{p=-k}^{k} D^k_{mp}(\boldsymbol{Q}^T)\boldsymbol{H}_p = \sum_{p=-k}^{k} D^{k,\pm}_{mp}(\boldsymbol{Q}^T)\boldsymbol{H}_p \tag{3.29}$$

for each $\boldsymbol{Q} = \boldsymbol{R} \in \mathrm{SO}(3)$.

Now for each $\boldsymbol{Q} = \boldsymbol{IR} \in \boldsymbol{I}\mathrm{SO}(3)$, it follows from (3.1), (3.2) and (3.25) that

$$
\begin{aligned}
\mathcal{T}_{\boldsymbol{Q}}\boldsymbol{H}_m &= \boldsymbol{Q}^{\otimes r}\boldsymbol{H}_m = (\boldsymbol{IR})^{\otimes r}\boldsymbol{H}_m \\
&= (-1)^r \sum_{p=-k}^{k} D^k_{mp}(\boldsymbol{R}^T)\boldsymbol{H}_p \\
&= \begin{cases} \displaystyle\sum_{p=-k}^{k} D^k_{mp}(\boldsymbol{R}^T)\boldsymbol{H}_p & \text{if } r \text{ is even} \\ \displaystyle -\sum_{p=-k}^{k} D^k_{mp}(\boldsymbol{R}^T)\boldsymbol{H}_p & \text{if } r \text{ is odd} \end{cases} \\
&= \begin{cases} \displaystyle\sum_{p=-k}^{k} D^{k,+}_{mp}(\boldsymbol{IR}^T)\boldsymbol{H}_p & \text{if } r \text{ is even} \\ \displaystyle\sum_{p=-k}^{k} D^{k,-}_{mp}(\boldsymbol{IR}^T)\boldsymbol{H}_p & \text{if } r \text{ is odd} \end{cases} \\
&= \begin{cases} \displaystyle\sum_{p=-k}^{k} D^{k,+}_{mp}(\boldsymbol{Q}^T)\boldsymbol{H}_p & \text{if } r \text{ is even} \\ \displaystyle\sum_{p=-k}^{k} D^{k,-}_{mp}(\boldsymbol{Q}^T)\boldsymbol{H}_p. & \text{if } r \text{ is odd.} \end{cases}
\end{aligned} \tag{3.30}
$$

Combining (3.29) and (3.30), we obtain (3.28) for material tensors.

For the case of pseudotensors, (3.28) can be proved by (3.27), together with (3.1), (3.2) and (3.24).

Theorem 3.3.3. *Let $Z \subset V^{\otimes r}$ be a subspace invariant under the action of the orthogonal group* O(3)*, and let Z_c be its complexification. For material tensors (reps. pseudotensors), which obey transformation law (2.38) (resp. (2.39)), Z_c is decomposed into its irreducible parts under* O(3) *as*

$$
Z_c = \begin{cases} n_0\mathcal{D}_0^+ + n_1\mathcal{D}_1^+ + \cdots + n_r\mathcal{D}_r^+ & \textit{if } r \textit{ is even (resp. odd)} \\ n_0\mathcal{D}_0^- + n_1\mathcal{D}_1^- + \cdots + n_r\mathcal{D}_r^- & \textit{if } r \textit{ is odd (resp. even)}, \end{cases} \tag{3.31}
$$

where the multiplicities n_k ($i = 0, 1, \cdots, r$) are exactly those that appear in the decomposition

$$Z_c = n_0\mathcal{D}_0 + n_1\mathcal{D}_1 + \cdots + n_r\mathcal{D}_r \tag{3.32}$$

under the rotation group SO(3)*, where some of the n_k's may be zero but $\sum_{k=0}^{r} n_k(2k+1) = \dim Z_c$. In the decomposition formula (3.31), $n_r \leq 1$; when $Z_c = V_c^{\otimes r}$, $n_r = 1$.*

Proof. Since SO(3) ⊂ O(3), Z_c is invariant under SO(3). Under SO(3), the decomposition of Z_c into its irreducible parts is of the form (3.32) [20, 28, 38], where the multiplicity n_k ($k = 0, 1, \cdots, r$) is the number of times that the irreducible representation $\mathcal{D}_k$ appears in the representation $\boldsymbol{R} \mapsto \boldsymbol{R}^{\otimes r}|Z_c$. By applying Lemma 3.3.1 to each irreducible invariant subspace of Z_c under SO(3), we obtain decomposition (3.31) of Z_c under O(3) for material tensors (reps. pseudotensors).

As for the last assertion of the theorem, it suffices to prove that $n_r = 1$ in (3.32) when $Z_c = V_c^{\otimes r}$, because the value of n_r in (3.31) is the same as that in (3.32) and the value of n_r in the decomposition of $V_c^{\otimes r}$ is clearly an upper bound for its counterpart in the decomposition of any of its invariant subspaces. Let χ_l and χ_ρ be the character of the irreducible representation $\mathcal{D}_l$ and of the representation $\boldsymbol{Q} \mapsto \boldsymbol{Q}^{\otimes r}$, respectively. Note that $\chi_l(\boldsymbol{R}(\boldsymbol{n},\omega)) = \sum_{k=-l}^{l} e^{\sqrt{-1}k\omega}$ ($l = 0, 1, \cdots$), $\chi_\rho(\boldsymbol{R}(\boldsymbol{n},\omega)) = (e^{\sqrt{-1}\omega} + 1 + e^{-\sqrt{-1}\omega})^r$, and $\chi_\rho = n_0\chi_0 + n_1\chi_1 + \cdots + n_r\chi_r$. Clearly n_r is equal to the coefficient of the term $e^{\sqrt{-1}r\omega}$ in $\chi_\rho(\boldsymbol{R}(\boldsymbol{n},\omega))$, which is 1. □

To specify the various types of tensors (or tensor spaces), let $V^{\otimes 2}$ be the tensor product $V \otimes V$, let $[V^{\otimes 2}]$ stand for the space of symmetric second-order tensors, and let $[[V^{\otimes 2}]^{\otimes 2}]$ denote the symmetric square of $[V^{\otimes 2}]$ (i.e., the symmetrized tensor product of $[V^{\otimes 2}]$ and $[V^{\otimes 2}]$) [20]. And we use the same notations for pseudotensors. Later in this study, we will apply the representation theorem to elasticity tensors (or stiffness tensor) $\boldsymbol{C}$, which are fourth-order tensors with the major and minor symmetries [11, 23]. Hence $\boldsymbol{C} \in [[V^{\otimes 2}]^{\otimes 2}]$, and $\boldsymbol{C}$ can be expressed in the Voigt notation [41] with 21 independent components as follows:

$$\boldsymbol{C} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ c_{12} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ c_{13} & c_{23} & c_{33} & c_{34} & c_{35} & c_{36} \\ c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} \\ c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} \\ c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66} \end{pmatrix}. \tag{3.33}$$

And tensors in $[[V_c^{\otimes 2}]^{\otimes 2}]$ can be decomposed into its irreducible parts under SO(3) as follows [20]:

$$[[V_c^{\otimes 2}]^{\otimes 2}] = 2\mathcal{D}_0 + 2\mathcal{D}_2 + \mathcal{D}_4. \tag{3.34}$$

Here the non-trivial multiplicities are: $n_0 = 2$, $n_2 = 2$, and $n_4 = 1$.

By Theorem 3.3.3, tensors in $[[V_c^{\otimes 2}]^{\otimes 2}]$ (e.g. fourth-order elasticity tensor) can be decomposed into its irreducible parts under O(3) as

$$[[V_c^{\otimes 2}]^{\otimes 2}] = 2\mathcal{D}_0^+ + 2\mathcal{D}_2^+ + \mathcal{D}_4^+. \tag{3.35}$$

For pseudotensors in $[[V_c^{\otimes 2}]^{\otimes 2}]$, the corresponding decomposition formula under O(3) is:

$$[[V_c^{\otimes 2}]^{\otimes 2}] = 2\mathcal{D}_0^- + 2\mathcal{D}_2^- + \mathcal{D}_4^-. \tag{3.36}$$

Chapter 4 Orientation measures on O(3) and the extended representation theorem

4.1 SO(3)-based classical texture analysis

In classical texture analysis, while material scientists usually characterize crystallographic texture by the orientation distribution functions (ODF), they also talk about ideal textures, where all crystallites have the same orientation, as limits of suitable sequences of ODFs. Mathematically it is more convenient to present classical texture analysis by using orientation measures [17, 21] as the starting point.

Let a reference crystal lattice be given. In classical texture analysis, the orientation of the crystal lattice at a sampling point X in a polycrystal is described by the rotation $\boldsymbol{R}(X)$ that brings the reference lattice to the lattice at X. The basic assumption is that there exists a positive Radon measure $\wp$, which is called the orientation (probability) measure [21] and satisfies $\wp(\mathrm{SO}(3)) = 1$, such that for each measurable set $\mathcal{A} \subset \mathrm{SO}(3)$, $\wp(\mathcal{A})$ gives the probability of finding $\boldsymbol{R}(X) \in \mathcal{A}$. When the orientation measure $\wp$ is absolutely continuous with respect to the volume measure $\mathcal{V} := 8\pi^2 g$, where g is the normalized Haar measure on SO(3), the Radon-Nikodym derivative $d\wp/d\mathcal{V}$ is well defined [12]. The function $w : \mathrm{SO}(3) \to \mathbb{R}$ defined by

$$w(\boldsymbol{R}) = \frac{d\wp}{d\mathcal{V}}(\boldsymbol{R}) \qquad \text{for each } \boldsymbol{R} \in \mathrm{SO}(3) \tag{4.1}$$

is the orientation distribution function (ODF) in classical texture analysis. In Roe's pioneering paper [32] on quantitative texture analysis, he takes ODFs as functions of the Euler angles and adopts the normalization

$$\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} w(\psi,\theta,\phi)\sin\theta\, d\psi d\theta d\phi = \int_{\mathrm{SO}(3)} w\, d\mathcal{V} = 1, \tag{4.2}$$

which has since become standard practice for materials scientists who follow Roe's approach in texture analysis.

When the ODF is square-integrable, i.e., $w \in L^2(\mathrm{SO}(3))$, it can be expanded (see [17] and the references therein) as an infinite series of Wigner D-functions $D^l_{mn} : \mathrm{SO}(3) \to \mathbb{C}$ (see (2.26)):

$$w(\boldsymbol{R}(\psi, \theta, \phi)) = \frac{1}{8\pi^2} + \sum_{l=1}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} c^l_{mn} D^l_{mn}(\boldsymbol{R}(\psi, \theta, \phi)), \tag{4.3}$$

where the Wigner D-functions satisfy (2.28), (2.29),

$$D^l_{mn}(\boldsymbol{R}) = (-1)^{m+n} \overline{D^l_{\bar{m}\bar{n}}(\boldsymbol{R})}, \tag{4.4}$$

where $\bar{m} = -m$ and $\bar{n} = -n$, and the orthogonality relations

$$\int_{\mathrm{SO}(3)} D^l_{mn}(\boldsymbol{R}) \overline{D^{l'}_{m'n'}(\boldsymbol{R})}\, d\mathcal{V} = \frac{8\pi^2}{2l+1} \delta_{ll'} \delta_{mm'} \delta_{nn'}. \tag{4.5}$$

As the ODF (w) is real-valued, the coefficients in the preceding expansion satisfy the following condition [18],

$$c^l_{mn} = (-1)^{m+n} \overline{c^l_{\bar{m}\bar{n}}}. \tag{4.6}$$

In Roe's notation [32], the series expansion of w is written in the form

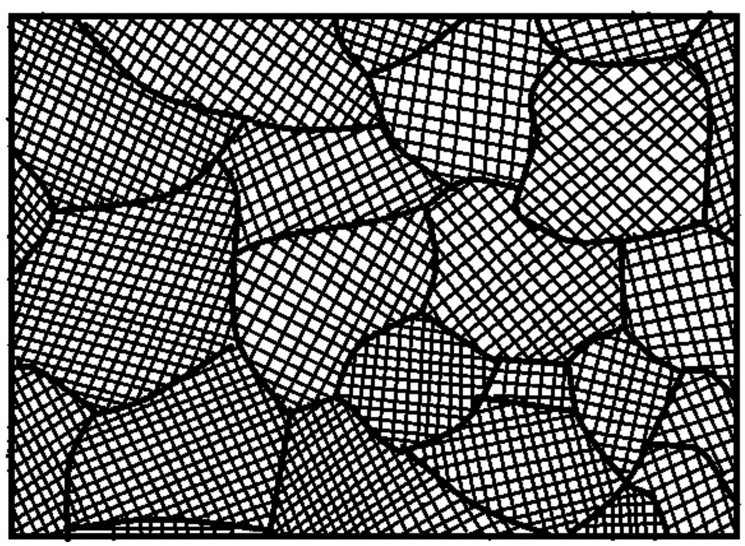
$$w(\boldsymbol{R}(\psi, \theta, \phi)) = \frac{1}{8\pi^2} + \sum_{l=1}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} W_{lmn} Z_{lmn}(\cos\theta) e^{-im\psi} e^{-in\theta}, \tag{4.7}$$

where

$$W_{lmn} = (-1)^{m-n} \sqrt{\frac{2}{2l+1}} c^l_{mn}, \qquad Z_{lmn}(\cos\theta) = (-1)^{m-n} \sqrt{\frac{2l+1}{2}} d^l_{mn}(\theta). \tag{4.8}$$

Central to the theory of texture analysis are [32, 33, 5, 17] the restrictions imposed on the ODF by texture (or sample) symmetry and crystal symmetry as defined by the groups G_{tex} and G_{cr}, respectively. These restrictions are derived through formulas that describe how the ODF transforms under rotation of sample and rotation of reference crystal lattice. Since all the classical restrictions and formulas in this regard will be subsumed by their counterparts in our O(3)-based theory, we refrain from saying more on them here.

Figure 4.1: A schematic figure of a polycrystalline aggregate



4.2 Orientation measures on O(3)

With ODFs defined on SO(3), classical texture analysis suffers from the limitation that the groups of texture and crystal symmetry G_{tex} and G_{cr} are restricted to be rotational. Thus, strictly speaking, all polycrystalline materials with G_{cr} being improper, which include most engineering materials (e.g., metals) with important applications, are not covered by the theory of classical texture analysis. That in applications of texture analysis substituting an improper G_{cr} by its proper peer in the same Laue class seems to have often worked does not validate such an ad hoc practice. On the contrary, such unexpected "successes" of the classical theory should be explained, and the conditions which render them possible delineated.

Bunge and his coworkers [5, 6, 7, 8] were the first to introduce ODFs that are defined on O(3). However, they stopped pursuing further after giving some basic properties of the ODF that include the restrictions imposed on it by texture and crystal symmetries and some discussions that concern its measurement by X-ray diffraction. Below we will cite their work whenever there is overlap with ours.

Henceforth we will assume that orientation probability measures $\wp$ are defined on O(3).

4.2.1 Orientation measures of single crystals

As illustration and for later use, we will write down the orientation measures of single crystals which belong to a Laue class that contains all three types of crystals. Let G_1, G_2, and G_3 be crystallographic point groups of Type I, Type II, and Type III in one such Laue class, respectively. By observation of Table 2.2, it is clear that we can represent the structure of each group as follows:

$$G_1 = G \cup \boldsymbol{R}G \qquad \text{where } \boldsymbol{R} \notin G \text{ and } G \text{ is a rotational point group;} \tag{4.9}$$

$$G_2 = G_1 \cup \boldsymbol{I}G_1 = G \cup \boldsymbol{R}G \cup \boldsymbol{I}G \cup \boldsymbol{IR}G; \tag{4.10}$$

$$G_3 = G \cup \boldsymbol{IR}G. \tag{4.11}$$

Let G have order N, and let $\boldsymbol{R}_k$ ($k = 1, \cdots, N$) be the elements of G. Then $\boldsymbol{RR}_k$ ($k = 1, \cdots, N$) are the elements of $\boldsymbol{R}G$. It follows that we can rewrite G_1 as:

$$G_1 = \{\boldsymbol{R}_1, \cdots, \boldsymbol{R}_N, \boldsymbol{RR}_1, \cdots, \boldsymbol{RR}_N\} = \{\boldsymbol{R}_1, \cdots, \boldsymbol{R}_N, \boldsymbol{R}_{N+1}, \cdots, \boldsymbol{R}_{2N}\} \tag{4.12}$$

where $\boldsymbol{R}_{N+1} = \boldsymbol{RR}_1, \cdots, \boldsymbol{R}_{2N} = \boldsymbol{RR}_N$.

It follows that G_2 and G_3 have the following elements:

$$G_2 = \{\boldsymbol{R}_1, \cdots, \boldsymbol{R}_N, \boldsymbol{R}_{N+1}, \cdots, \boldsymbol{R}_{2N}, \boldsymbol{IR}_1, \cdots \boldsymbol{IR}_N, \boldsymbol{IR}_{N+1}, \cdots, \boldsymbol{IR}_{2N}\} \tag{4.13}$$

$$G_3 = \{\boldsymbol{R}_1, \cdots \boldsymbol{R}_N, \boldsymbol{IR}_{N+1}, \cdots, \boldsymbol{IR}_{2N}\} \tag{4.14}$$

Let $\delta_{\boldsymbol{Q}}$ be the Dirac measure at $\boldsymbol{Q} \in \mathrm{O}(3)$, i.e., for all measurable $\mathcal{A} \subset \mathrm{O}(3)$,

$$\delta_{\boldsymbol{Q}}(\mathcal{A}) = \begin{cases} 1 & \text{if } \boldsymbol{Q} \in \mathcal{A} \\ 0 & \text{if } \boldsymbol{Q} \notin \mathcal{A} \end{cases}. \tag{4.15}$$

Consider a single crystal with point group G_1 whose orientation with respect to the chosen reference lattice is specified by a rotation $\boldsymbol{R}_0$. The orientation measure of the single crystal is [21]:

$$\wp_1 = \frac{1}{2N} \sum_{i=1}^{2N} \delta_{\boldsymbol{R}_0 \boldsymbol{R}_i}. \tag{4.16}$$

Similarly, if the single crystal has symmetry group G_2, its orientation measure is given by

$$\wp_2 = \frac{1}{4N} \left(\sum_{i=1}^{2N} \delta_{\boldsymbol{R}_0 \boldsymbol{R}_i} + \sum_{i=1}^{2N} \delta_{\boldsymbol{I}\boldsymbol{R}_0 \boldsymbol{R}_i} \right). \tag{4.17}$$

If the single crystal has symmetry group G_3, its orientation measure is:

$$\wp_3 = \frac{1}{2N}\left(\sum_{i=1}^{N} \delta_{\boldsymbol{R}_0\boldsymbol{R}_i} + \sum_{i=N+1}^{2N} \delta_{\boldsymbol{I}\boldsymbol{R}_0\boldsymbol{R}_i}\right). \tag{4.18}$$

4.2.2 Transformation formulas for orientation measures. Texture and crystal symmetries

Let $\wp$ and $\mathcal{T}_{\boldsymbol{R}}\wp$ be the orientation measure of a polycrystal before and after it undergoes a rotation $\boldsymbol{R} \in \mathrm{SO}(3)$, respectively. For each measurable $\mathcal{A} \subset \mathrm{SO}(3)$, clearly we have

$$(\mathcal{T}_{\boldsymbol{R}}\wp)(\mathcal{A}) = \wp(\boldsymbol{R}^T\mathcal{A}), \tag{4.19}$$

where $\boldsymbol{R}^T\mathcal{A} = \{\boldsymbol{R}^T\boldsymbol{P} : \boldsymbol{P} \in \mathcal{A}\}$. In the context of classical texture analysis, transformation formula (4.19) can be traced back to Roe's 1965 paper [32], where it is expressed in terms of the ODF.

Here we allow polycrystals to undergo also roto-inversions, and we extend (4.19) as follows. Let $\wp$ and $\mathcal{T}_{\boldsymbol{Q}}\wp$ be the orientation measure of a polycrystal before and after it undergoes a rotation or roto-inversion $\boldsymbol{Q} \in \mathrm{O}(3)$, respectively. For each measurable $\mathcal{A} \subset \mathrm{O}(3)$, we have

$$(\mathcal{T}_{\boldsymbol{Q}}\wp)(\mathcal{A}) = \wp(\boldsymbol{Q}^T\mathcal{A}), \tag{4.20}$$

where $\boldsymbol{Q}^T\mathcal{A} = \{\boldsymbol{Q}^T\boldsymbol{P} : \boldsymbol{P} \in \mathcal{A}\}$. The subgroup G_{tex} of elements $\boldsymbol{Q} \in \mathrm{O}(3)$ that observe

$$\mathcal{T}_{\boldsymbol{Q}}\wp = \wp \tag{4.21}$$

is the group of texture (or sample) symmetry of the polycrystal.

Likewise, let $\wp$ and $\widetilde{\mathcal{T}}_{\boldsymbol{Q}}\wp$ be the orientation measure of a polycrystal before and after the reference crystal lattice undergoes a rotation or roto-inversion $\boldsymbol{Q} \in \mathrm{O}(3)$, respectively. For each measurable $\mathcal{A}$, clearly we have

$$(\widetilde{\mathcal{T}}_{\boldsymbol{Q}}\wp)(\mathcal{A}) = \wp(\mathcal{A}\boldsymbol{Q}), \tag{4.22}$$

where $\mathcal{A}\boldsymbol{Q} = \{\boldsymbol{QP} : \boldsymbol{P} \in \mathcal{A}\}$. The subgroup G_{cr} of elements $\boldsymbol{Q} \in \text{SO}(3)$ that observe

$$\widetilde{\mathcal{T}}_{\boldsymbol{Q}}\wp = \wp \tag{4.23}$$

is the group of crystal symmetry.

Figure 4.2: Images of left- and right-handed quartz

4.2.3 Enantiomorphism. Right-handed and left-handed crystals

Type I crystals are enantiomorphic. They can exist in right- and left-handed forms (see Figure 4.2 [1]). Under inversion, a right-handed crystal becomes a left-handed crystal, and vice versa. By transformation formula (4.20), we see that

$$\mathcal{T}_{\boldsymbol{I}}\delta_{\boldsymbol{R}} = \delta_{\boldsymbol{IR}}, \qquad \mathcal{T}_{\boldsymbol{I}}\delta_{\boldsymbol{IR}} = \delta_{\boldsymbol{R}} \qquad \text{for each } \boldsymbol{R} \in \mathrm{SO}(3). \tag{4.24}$$

Hence we can and we will adopt the convention that right-handed and left-handed Type 1 crystals have the support of their orientation measures in SO(3) and $\boldsymbol{I}$SO(3), respectively.

A polycrystal which consists of both right- and left-handed crystallites has the support of its orientation measure in both SO(3) and $\boldsymbol{I}$SO(3). Let $\lambda, (1-\lambda) \in [0,1]$ be the volume fraction of right- and left-handed crystallites in the polycrystal, respectively. Under inversion, the volume fractions of right- and left-handed crystallites in the polycrystal become $1-\lambda$ and λ, respectively. The proportion of right- and left-handed crystallites in the polycrystal will not change under inversion if and only if $\lambda = 1/2$.

Consider a single crystal of Type II. It has a point group of the form $G \cup \boldsymbol{I}G$, where G is a rotational point group. Let $G = \{\boldsymbol{R}_1, \cdots, \boldsymbol{R}_N\}$, and let the orientation of the given single crystal with respect to a chosen reference lattice be specified by a rotation $\boldsymbol{R}_0$. The orientation measure of the Type II crystal in question is then given by

$$\wp = \frac{1}{2N}\left(\sum_{i=1}^{N} \delta_{\boldsymbol{R}_0\boldsymbol{R}_i} + \sum_{i=1}^{N} \delta_{\boldsymbol{I}\boldsymbol{R}_0\boldsymbol{R}_i}\right). \tag{4.25}$$

Since $\wp(\mathrm{SO}(3)) = \wp(\boldsymbol{I}\mathrm{SO}(3)) = 1/2$, we may take a Type II crystal as a mixture of right- and left-handed crystallites in equal volume fractions. Moreover, from (4.25) we clearly have

$$\mathcal{T}_{\boldsymbol{I}}\wp = \wp. \tag{4.26}$$

[1] I am indebted to Dr. S.F. Pavkovic for granting me his permission to reproduce this figure.

Thus, from the standpoint of texture analysis, we may regard a Type II crystal as a special type of mixture of right- and left-handed crystallites that is invariant under inversion. It is also apparent that (4.26) remains valid for the orientation measure of any polycrystalline aggregate of Type II crystallites.

Each single crystal of Type III has a point group of the form $G \cup \boldsymbol{IR}G$. While its orientation measure $\wp$ is not invariant under inversion, it still satisfies

$$\wp(\mathrm{SO}(3)) = \wp(\boldsymbol{I}\mathrm{SO}(3)) = \frac{1}{2}. \tag{4.27}$$

Thus, from the standpoint of texture analysis, we may take a Type III single crystal as a mixture of right- and left-handed crystallites in equal volume fractions.

4.3 Orientation distribution functions on O(3)

When the orientation measure $\wp$ is absolutely continuous with respect to the volume measure $\mathcal{V}$ on O(3) (see Section 2.2.3), the Radon-Nikodym derivative $d\wp/d\mathcal{V}$ is well defined. The function $w : \mathrm{O}(3) \to \mathbb{R}^1$ defined by

$$w(\boldsymbol{Q}) = \frac{d\wp}{d\mathcal{V}}(\boldsymbol{Q}) \qquad \text{for each } \boldsymbol{Q} \in \mathrm{O}(3) \tag{4.28}$$

is the orientation distribution function (ODF). Since the ODFs are [30] dense in the space of orientation measures (i.e., positive Radon measures $\wp$ on O(3) with $\wp(\mathrm{O}(3)) = 1$) under the weak* topology, there is no loss in generality to work with ODFs instead of orientation measures.

All the basic concepts and formulas introduced above through orientation measures can be easily translated into their counterparts in terms of ODFs. For example, let w be the ODF that characterizes the texture of a given polycrystal. Let $\mathcal{T}_{\boldsymbol{Q}}w$ and $\widetilde{\mathcal{T}}_{\boldsymbol{Q}}w$ be the ODF of the polycrystal after it undergoes a rotation or roto-inversion and after the reference lattice undergoes undergoes a rotation or roto-inversion $\boldsymbol{Q} \in \mathrm{O}(3)$, respectivelyy. Parallel to (4.20) and (4.22), we have

$$(\mathcal{T}_{\boldsymbol{Q}} w)(\boldsymbol{P}) = w(\boldsymbol{Q}^T \boldsymbol{P}) \qquad \text{for each } \boldsymbol{P} \in \mathrm{O}(3), \tag{4.29}$$

and

$$(\widetilde{\mathcal{T}}_{\boldsymbol{Q}} w)(\boldsymbol{P}) = w(\boldsymbol{P}\boldsymbol{Q}) \qquad \text{for each } \boldsymbol{P} \in \mathrm{O}(3). \tag{4.30}$$

The groups of texture symmetry and crystal symmetry are defined respectively as follows:

$$G_{\text{tex}} = \{\boldsymbol{Q} \in \mathrm{O}(3) : \mathcal{T}_{\boldsymbol{Q}} w = w\}, \tag{4.31}$$

$$G_{\text{cr}} = \{\boldsymbol{Q} \in \mathrm{O}(3) : \widetilde{\mathcal{T}}_{\boldsymbol{Q}} w = w\}. \tag{4.32}$$

Since O(3) is the disjoint union of SO(3) and $\boldsymbol{I}$SO(3), we can take an ODF defined on O(3) as a pair of functions, each of which is defined on SO(3).

Definition 4.3.1. [8] *Let* $w : \mathrm{O}(3) \to \mathbb{R}^1$ *be the ODF. Define* $w^{R/L} : \mathrm{SO}(3) \to \mathbb{R}^1$ *by*

$$w^R(\boldsymbol{R}) = w(\boldsymbol{R}), \qquad w^L(\boldsymbol{R}) = w(\boldsymbol{I}\boldsymbol{R}), \qquad \textit{for } \boldsymbol{R} \in \mathrm{SO}(3). \tag{4.33}$$

By transformation formula (4.29), we have

$$\mathcal{T}_{\boldsymbol{I}} w(\boldsymbol{P}) = w(\boldsymbol{I}^{-1}\boldsymbol{P}) = w(\boldsymbol{I}\boldsymbol{P}) \quad \text{for } \boldsymbol{P} \in \mathrm{O}(3); \tag{4.34}$$

here $\mathcal{T}_{\boldsymbol{I}} w(\boldsymbol{P})$ denotes the ODF after inversion $\boldsymbol{I}$ of the polycrystal. It follows then from Definition (4.3.1) that

$$(\mathcal{T}_{\boldsymbol{I}} w)^R(\boldsymbol{R}) = (\mathcal{T}_{\boldsymbol{I}} w)(\boldsymbol{R}) = w(\boldsymbol{I}\boldsymbol{R}) = w^L(\boldsymbol{R}) \quad \text{for } \boldsymbol{R} \in \mathrm{SO}(3), \tag{4.35}$$

and

$$(\mathcal{T}_{\boldsymbol{I}} w)^L(\boldsymbol{R}) = (\mathcal{T}_{\boldsymbol{I}} w)(\boldsymbol{I}\boldsymbol{R}) = w(\boldsymbol{R}) = w^R(\boldsymbol{R}) \quad \text{for } \boldsymbol{R} \in \mathrm{SO}(3). \tag{4.36}$$

The ODF w is determined by the pair (w^R, w^L) and vice versa. The ODF (w^R, w^L) of an aggregate of right-handed crystallites can be written as $(w^R, w^L) = (w_o, 0)$ for some $w_o : \mathrm{SO}(3) \to \mathbb{R}^1$. Under inversion, each right-handed crystallite becomes a left-handed crystallite. The ODF of the aggregate becomes $((\mathcal{T}_{\boldsymbol{I}} w)^R, (\mathcal{T}_{\boldsymbol{I}} w)^L) = (0, w_o)$.

Each improper group of Type II is of the form $G = G_p \cup \boldsymbol{I} G_p$, where G_p is a rotational point group. For example, $O_h = O \cup \boldsymbol{I}O$, $D_{6h} = D_6 \cup \boldsymbol{I}D_6$. Because $\boldsymbol{I} \in G_{\mathrm{cr}}$, the group of crystal symmetry, by (4.30), (4.32), and Definition 4.3.1 we have

$$w^R(\boldsymbol{R}) = w(\boldsymbol{R}) = w(\boldsymbol{RI}) = w(\boldsymbol{IR}) = w^L(\boldsymbol{R}) \quad \text{for each } \boldsymbol{R} \in \mathrm{SO}(3). \tag{4.37}$$

We record this simple but important observation as a proposition.

Proposition 4.3.2. *The right- and left-handed parts w^R and w^L of the ODF w of any polycrystalline aggregate of Type II crystallites are identical.*

4.3.1 Series expansions and texture coefficients

By Theorem 3.1.1 and the theory of group representations [28], each orientation distribution function $w \in L^2(\mathrm{O}(3))$ can be expanded as an infinite series in terms of the matrix elements $D^{l,\pm}_{mn}$ of the complete set of irreducible unitary representations $\mathcal{D}^{l,\pm}$ of O(3):

$$w(\boldsymbol{Q}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} c^{l,+}_{mn} D^{l,+}_{mn}(\boldsymbol{Q}) + \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} c^{l,-}_{mn} D^{l,-}_{mn}(\boldsymbol{Q}) \tag{4.38}$$

$$= \begin{cases} \displaystyle\sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} (c^{l,+}_{mn} + c^{l,-}_{mn}) D^{l}_{mn}(\boldsymbol{R}(\psi, \theta, \phi)) & \text{for } \boldsymbol{Q} = \boldsymbol{R} \in \mathrm{SO}(3) \\ \displaystyle\sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} (c^{l,+}_{mn} - c^{l,-}_{mn}) D^{l}_{mn}(\boldsymbol{R}(\psi, \theta, \phi)) & \text{for } \boldsymbol{Q} = \boldsymbol{IR} \in \boldsymbol{I}\mathrm{SO}(3), \end{cases} \tag{4.39}$$

where the expansion coefficients are called texture coefficients and they satisfy

$$c^{l,\pm}_{mn} = (-1)^{m+n} \overline{c^{l,\pm}_{\bar{m}\bar{n}}}. \tag{4.40}$$

Let w_0 be an ODF which has all its texture coefficients with $l \geq 1$ vanish. By (4.38), we have

$$w_0 = w_0(\boldsymbol{Q}) = c_{00}^{0,+} D_{00}^{0,+}(\boldsymbol{Q}) + c_{00}^{0,-} D_{00}^{0,-}(\boldsymbol{Q}) \tag{4.41}$$

where $D_{00}^{0,+}(\boldsymbol{Q}) = D_{00}^{0}(\boldsymbol{R}) = 1$ for any $\boldsymbol{Q} \in \mathrm{O}(3)$, and

$$D_{00}^{0,-}(\boldsymbol{Q}) = \begin{cases} D_{00}^{0}(\boldsymbol{R}) = 1 & \text{for } \boldsymbol{Q} = \boldsymbol{R} \in \mathrm{SO}(3) \\ -D_{00}^{0}(\boldsymbol{R}) = -1 & \text{for } \boldsymbol{Q} = \boldsymbol{I}\boldsymbol{R} \in \boldsymbol{I}\mathrm{SO}(3). \end{cases} \tag{4.42}$$

It follows that

$$w_0(\boldsymbol{Q}) = \begin{cases} c_{00}^{0,+} + c_{00}^{0,-} & \text{for } \boldsymbol{Q} \in \mathrm{SO}(3) \\ c_{00}^{0,+} - c_{00}^{0,-} & \text{for } \boldsymbol{Q} \in \boldsymbol{I}\mathrm{SO}(3). \end{cases} \tag{4.43}$$

and from the normalization condition we have

$$\begin{aligned} 1 &= \int_{\mathrm{O}(3)} w_0 \, d\mathcal{V} \\ &= \int_{\mathrm{SO}(3)} (c_{00}^{0,+} + c_{00}^{0,-}) \, d\mathcal{V} + \int_{\boldsymbol{I}\mathrm{SO}(3)} (c_{00}^{0,+} - c_{00}^{0,-}) \, d\mathcal{V} \\ &= 8\pi^2 (c_{00}^{0,+} + c_{00}^{0,-}) + 8\pi^2 (c_{00}^{0,+} - c_{00}^{0,-}) \\ &= 16\pi^2 c_{00}^{0,+}, \end{aligned} \tag{4.44}$$

which implies $c_{00}^{0,+} = \dfrac{1}{16\pi^2}$. Clearly the normalization condition does not put any restriction on $c_{00}^{0,-}$. It turns out that the coefficient $c_{00}^{0,-}$ is determined by the volume fraction of right-handed crystallites in the polycrystal as we shall see.

By Definition (4.3.1) regarding w^R and w^L, we have

$$w(\boldsymbol{Q}) = \begin{cases} w^R(\boldsymbol{R}) = \displaystyle\sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} c_{mn}^{l,R} D_{mn}^{l}(\boldsymbol{R}(\psi, \theta, \phi)) & \text{for } \boldsymbol{Q} = \boldsymbol{R} \in \mathrm{SO}(3) \\ w^L(\boldsymbol{R}) = \displaystyle\sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} c_{mn}^{l,L} D_{mn}^{l}(\boldsymbol{R}(\psi, \theta, \phi)) & \text{for } \boldsymbol{I}\boldsymbol{Q} = \boldsymbol{R} \in \mathrm{SO}(3). \end{cases} \tag{4.45}$$

Combining (4.39) and (4.45), we have,

$$c_{mn}^{l,R} = c_{mn}^{l,+} + c_{mn}^{l,-}, \qquad c_{mn}^{l,L} = c_{mn}^{l,+} - c_{mn}^{l,-}. \tag{4.46}$$

And thus

$$c_{mn}^{l,+} = \frac{1}{2}(c_{mn}^{l,R} + c_{mn}^{l,L}), \qquad c_{mn}^{l,-} = \frac{1}{2}(c_{mn}^{l,R} - c_{mn}^{l,L}). \tag{4.47}$$

When $l = 0$, by (4.46) we have

$$c_{00}^{0,R} = c_{00}^{0,+} + c_{00}^{0,-}, \qquad c_{00}^{0,L} = c_{00}^{0,+} - c_{00}^{0,-}. \tag{4.48}$$

Substituting $c_{00}^{0,+} = \frac{1}{16\pi^2}$ into (4.48), we obtain

$$c_{00}^{0,R} = \frac{1}{16\pi^2} + c_{00}^{0,-}, \qquad c_{00}^{0,L} = \frac{1}{16\pi^2} - c_{00}^{0,-}. \tag{4.49}$$

Now let λ and $1-\lambda \in [0,1]$ be the volume fraction of right- and left-handed crystallites in the polycrystalline aggregate. We then have

$$c_{00}^{0,R} = \frac{1}{16\pi^2} + c_{00}^{0,-} = \frac{\lambda}{8\pi^2}, \qquad c_{00}^{0,L} = \frac{1}{16\pi^2} - c_{00}^{0,-} = \frac{1-\lambda}{8\pi^2}. \tag{4.50}$$

Solving for $c_{00}^{0,-}$, we obtain $c_{00}^{0,-} = \dfrac{2\lambda - 1}{16\pi^2}$.

For $\lambda \in [0,1]$, let

$$\begin{aligned} w_{0,\lambda}(\boldsymbol{Q}) &= \frac{1}{16\pi^2} D_{00}^{0,+}(\boldsymbol{Q}) + \left(\frac{\lambda}{8\pi^2} - \frac{1}{16\pi^2}\right) D_{00}^{0,-}(\boldsymbol{Q}) \qquad \text{for } \boldsymbol{Q} \in \mathrm{O}(3) \\ &= \begin{cases} \dfrac{\lambda}{8\pi^2} & \text{for } \boldsymbol{Q} \in \mathrm{SO}(3) \\ \dfrac{1-\lambda}{8\pi^2} & \text{for } \boldsymbol{Q} \in \boldsymbol{I}\mathrm{SO}(3) \end{cases} \end{aligned} \tag{4.51}$$

be the ODF which pertains to an aggregate of right- and left-handed crystallites with volume fractions λ and $1-\lambda$, respectively, that has all texture coefficients with $l \geq 1$ equal to zero.

Remark: When $c_{00}^{0,-} = \frac{1}{16\pi^2}$, we have $\lambda = 1$, $c_{00}^{0,R} = \frac{1}{8\pi^2}$, while $c_{00}^{0,L} = 0$, i.e, the polycrystal consists of right-handed crystals. When $c_{00}^{0,-} = -\frac{1}{16\pi^2}$, we have $\lambda = 0$, $c_{00}^{0,R} = 0$, while

$c^{0,L}_{00} = \frac{1}{8\pi^2}$, i.e, the polycrystal consists of left-handed crystals. When $c^{0,-}_{00} = 0$, we have $\lambda = \frac{1}{2}$, $c^{0,R}_{00} = c^{0,L}_{00} = \frac{1}{16\pi^2}$, i.e, the polycrystal consists of half of right-handed crystals and half of left-handed crystals. Next we will discuss the case with $\lambda = \frac{1}{2}$ more for aggregates of Type II and Type III crystallites.

Proposition 4.3.3. *The ODF $w_{0,\lambda}$ is isotropic, i.e., it satisfies $\mathcal{T}_{\boldsymbol{Q}} w_{0,\lambda} = w_{0,\lambda}$ for each $\boldsymbol{Q} \in$ O(3) if and only if $c^{0,-}_{00} = 0$ or $\lambda = \frac{1}{2}$.*

Proof. Suppose $\mathcal{T}_{\boldsymbol{Q}} w_{0,\lambda} = w_{0,\lambda}$ for each $\boldsymbol{Q} \in$ O(3). For $\boldsymbol{Q} = \boldsymbol{I}$, we have

$$\begin{aligned}\mathcal{T}_{\boldsymbol{I}} w_{0,\lambda}(\boldsymbol{Q}_1) &= w_{0,\lambda}(\boldsymbol{I}^T\boldsymbol{Q}_1) = c^{0,+}_{00} D^{0,+}_{00}(\boldsymbol{I}^T\boldsymbol{Q}_1) + c^{0,-}_{00} D^{0,-}_{00}(\boldsymbol{I}^T\boldsymbol{Q}_1) \\ &= c^{0,+}_{00} D^{0,+}_{00}(\boldsymbol{I}^T) D^{0,+}_{00}(\boldsymbol{Q}_1) + c^{0,-}_{00} D^{0,-}_{00}(\boldsymbol{I}^T) D^{0,-}_{00}(\boldsymbol{Q}_1) \\ &= \begin{cases} c^{0,+}_{00} - c^{0,-}_{00} & \text{for } \boldsymbol{Q}_1 \in \mathrm{SO}(3) \\ c^{0,+}_{00} + c^{0,-}_{00} & \text{for } \boldsymbol{Q}_1 \in \boldsymbol{I}\mathrm{SO}(3). \end{cases}\end{aligned} \tag{4.52}$$

Comparing the preceding equation with (4.43), we conclude that $c^{0,-}_{00} = 0$, which is equivalent to $\lambda = \frac{1}{2}$.

Conversely, suppose $c^{0,-}_{00} = 0$. It follows then from (4.43) and (4.52) that $\mathcal{T}_{\boldsymbol{I}} w_{0,\lambda} = w_{0,\lambda}$. On the other hand, for each $\boldsymbol{R} \in$ SO(3) we have

$$\mathcal{T}_{\boldsymbol{R}} w_{0,\lambda}(\boldsymbol{Q}) = w_{0,\lambda}(\boldsymbol{R}^T\boldsymbol{Q}) = c^{0,+}_{00} D^{0,+}_{00}(\boldsymbol{R}^T) D^{0,+}_{00}(\boldsymbol{Q}) = c^{0,+}_{00} D^{0,+}_{00}(\boldsymbol{Q}) = w_0(\boldsymbol{Q}) \tag{4.53}$$

for each $\boldsymbol{Q} \in$ O(3). □

Henceforth we shall denote by w_{iso} the isotropic ODF $w_{0,\frac{1}{2}}$, which has all its texture coefficients vanish, i.e.,

$$w_{\text{iso}}(\boldsymbol{Q}) = \frac{1}{16\pi^2} \qquad \text{for each } \boldsymbol{Q} \in \mathrm{O}(3). \tag{4.54}$$

For aggregates of Type II and of Type III crystallites, we have the normalization conditions

$$\int_{\mathrm{SO}(3)} w^R(\boldsymbol{R})\, d\mathcal{V} = \frac{1}{2}, \qquad \int_{\mathrm{SO}(3)} w^L(\boldsymbol{R})\, d\mathcal{V} = \frac{1}{2}. \tag{4.55}$$

Parallel to the series expansion (4.3) for aggregates of Type I crystallites, we have

$$w^{R/L}(\boldsymbol{R}(\psi,\theta,\phi)) = \frac{1}{16\pi^2} + \sum_{l=1}^{\infty}\sum_{m=-l}^{l}\sum_{n=-l}^{l} c_{mn}^{l,R/L} D_{mn}^{l}(\boldsymbol{R}(\psi,\theta,\phi)) \tag{4.56}$$

for aggregates of Type II and of Type III crystallites.

4.4 Main assumption

The main assumption behind Man and Huang's proof of their representation theorem [20] is as follows: For each rotation $\boldsymbol{R}$, each rth-order material tensor $\boldsymbol{H}$, and each ODF w : $\mathrm{SO}(3) \to \mathbb{R}^1$, there holds

$$\boldsymbol{R}^{\otimes r}\boldsymbol{H}(w) = \boldsymbol{H}(\mathcal{T}_{\boldsymbol{R}} w), \tag{4.57}$$

where $\boldsymbol{R}^{\otimes r}(H_{i_1\cdots i_r}(w)\boldsymbol{e}_{i_1} \otimes \cdots \otimes \boldsymbol{e}_{i_r}) = H_{i_1\cdots i_r}(w)\boldsymbol{R}\boldsymbol{e}_{i_1} \otimes \cdots \otimes \boldsymbol{R}\boldsymbol{e}_{i_r}$. As a concrete example of a tensor function $\boldsymbol{H}(\cdot)$ that satisfies (4.57), consider the orientational average [20] of a specific r-th order tensor $\boldsymbol{H}_0$ defined by

$$\boldsymbol{H}(w) = 8\pi^2 \int_{\mathrm{SO}(3)} \boldsymbol{Q}^{\otimes r}\boldsymbol{H}_0 w(\boldsymbol{Q}) dg(\boldsymbol{Q}). \tag{4.58}$$

By appealing to the bi-invariance of the Haar measure, we have

$$\begin{aligned}
\boldsymbol{R}^{\otimes r}\boldsymbol{H}(w) &= 8\pi^2 \int_{\mathrm{SO}(3)} \boldsymbol{R}^{\otimes r}\boldsymbol{Q}^{\otimes r}\boldsymbol{H}_0 w(\boldsymbol{Q})dg(\boldsymbol{Q}) \\
&= 8\pi^2 \int_{\mathrm{SO}(3)} (\boldsymbol{R}\boldsymbol{Q})^{\otimes r}\boldsymbol{H}_0 w(\boldsymbol{Q})dg(\boldsymbol{Q}) \\
&= 8\pi^2 \int_{\mathrm{SO}(3)} \tilde{\boldsymbol{Q}}^{\otimes r}\boldsymbol{H}_0 w(\boldsymbol{R}^T\tilde{\boldsymbol{Q}})dg(\boldsymbol{R}^T\tilde{\boldsymbol{Q}}) \\
&= 8\pi^2 \int_{\mathrm{SO}(3)} \tilde{\boldsymbol{Q}}^{\otimes r}\boldsymbol{H}_0 w(\boldsymbol{R}^T\tilde{\boldsymbol{Q}})dg(\tilde{\boldsymbol{Q}}) \\
&= 8\pi^2 \int_{\mathrm{SO}(3)} \tilde{\boldsymbol{Q}}^{\otimes r}\boldsymbol{H}_0 \mathcal{T}_{\boldsymbol{R}} w(\tilde{\boldsymbol{Q}})dg(\tilde{\boldsymbol{Q}}) \\
&= \boldsymbol{H}(\mathcal{T}_{\boldsymbol{R}} w), \qquad (4.59)
\end{aligned}$$

where $\tilde{\boldsymbol{Q}} = \boldsymbol{R}\boldsymbol{Q}$.

Here we extend Man and Huang's assumption as follows: For each $\boldsymbol{Q} \in \mathrm{O}(3)$, each rth-order material tensor or pseudotensor $\boldsymbol{H}$, and each ODF $w : \mathrm{O}(3) \to \mathbb{R}^1$, there holds

$$\mathcal{T}_{\boldsymbol{Q}}\boldsymbol{H}(w) = \boldsymbol{H}(\mathcal{T}_{\boldsymbol{Q}} w). \qquad (4.60)$$

where $\mathcal{T}_{\boldsymbol{Q}}\boldsymbol{H} = \boldsymbol{Q}^{\otimes r}\boldsymbol{H}$ if $\boldsymbol{H}$ is a material tensor and $\mathcal{T}_{\boldsymbol{Q}}\boldsymbol{H} = (\det \boldsymbol{Q})\boldsymbol{Q}^{\otimes r}\boldsymbol{H}$ if $\boldsymbol{H}$ is a material pseudotensor, and $(\mathcal{T}_{\boldsymbol{Q}} w)(\boldsymbol{P}) = w(\boldsymbol{Q}^T\boldsymbol{P})$ for each $\boldsymbol{P} \in \mathrm{O}(3)$. Requirement (4.60) is the main physical assumption of the present study. It is equivalent to (4.57) amended by the requirement

$$\mathcal{T}_{\boldsymbol{I}}\boldsymbol{H}(w) = \boldsymbol{H}(\mathcal{T}_{\boldsymbol{I}} w). \qquad (4.61)$$

Before we apply our main assumption (4.60) in Section 4.6 to obtain a representation theorem for material tensors and pseudotensors that pertain to aggregates of Type II and Type III crystallites, we illustrate some of its non-trivial implications below.

Consider an rth-order tensor $\boldsymbol{H}$ pertaining to an aggregate of right-handed crystals with $(w^R, w^L) = (w_o, 0)$. By(2.40), (4.35), (4.36), and (4.61), the corresponding tensor of the left-handed counterpart with $(w^R, w^L) = (0, w_o)$ is given by

$$\begin{aligned} \boldsymbol{H}(0, w_o) &= \boldsymbol{H}(\mathcal{T}_{\boldsymbol{I}}(w_o, 0)) = \mathcal{T}_{\boldsymbol{I}}\boldsymbol{H}(w_o, 0) \\ &= (-1)^r \boldsymbol{H}(w_o, 0) = \begin{cases} \boldsymbol{H}(w_o, 0) & \text{for even } r; \\ -\boldsymbol{H}(w_o, 0) & \text{for odd } r. \end{cases} \end{aligned} \tag{4.62}$$

For an rth-order pseudotensor $\boldsymbol{H}$, with (2.41), we have instead

$$\begin{aligned} \boldsymbol{H}(0, w_o) &= \boldsymbol{H}(\mathcal{T}_{\boldsymbol{I}}(w_o, 0)) = \mathcal{T}_{\boldsymbol{I}}\boldsymbol{H}(w_o, 0) \\ &= (-1)^{r+1} \boldsymbol{H}(w_o, 0) = \begin{cases} -\boldsymbol{H}(w_o, 0) & \text{for even } r; \\ \boldsymbol{H}(w_o, 0) & \text{for odd } r. \end{cases} \end{aligned} \tag{4.63}$$

As illustration, let us apply (4.62) and (4.63) to the quartz crystal, which is enantiomorphic. Let $\boldsymbol{C}^L$, $\boldsymbol{E}^L$, $\boldsymbol{G}^L$ and $\boldsymbol{C}^R$, $\boldsymbol{E}^R$, $\boldsymbol{G}^R$ be the 4th-order elasticity tensor, the 3rd-order piezoelectric tensor, the 2nd-order gyration pseudotensor that pertain to the left- and right-handed (single) quartz crystal (see Figure 4.2), respectively. From (4.62) and (4.63), we get $\boldsymbol{C}^L = \boldsymbol{C}^R, \quad \boldsymbol{E}^L = -\boldsymbol{E}^R, \quad \boldsymbol{G}^L = -\boldsymbol{G}^R$. Cf. Figure 4.3, which is taken from *IEEE Standard on Piezoelectricity (176-1987)*; in the table c^E is the 4th-order elasticity tensor, and e is the 3rd-order piezoelectric tensor.

As shown in the following proposition, requirement (4.61) imposes strong restrictions on some classes of material tensors and pseudotensors.

Proposition 4.4.1. *Let $\boldsymbol{H}(w)$ be a material tensor (resp. pseudotensor) pertaining to a polycrystalline aggregate of Type II crystallites. Then $\boldsymbol{H}(w) = \boldsymbol{0}$ if it is of odd (resp. even) order.*

Proof. As $\boldsymbol{I} \in G_{\mathrm{cr}}$, $\boldsymbol{I}^{-1} = \boldsymbol{I}$, and $\boldsymbol{QI} = \boldsymbol{IQ}$ for $\boldsymbol{Q} \in \mathrm{O}(3)$, we have

$$(\mathcal{T}_{\boldsymbol{I}} w)(\boldsymbol{Q}) = w(\boldsymbol{I}^{-1}\boldsymbol{Q}) = w(\boldsymbol{IQ}) = w(\boldsymbol{QI}) = w(\boldsymbol{Q}) \quad \text{for each } \boldsymbol{Q} \in \mathrm{O}(3).$$

It then follows from (4.61), (2.40), and (2.41) that

$$\boldsymbol{H}(w) = \boldsymbol{H}(\mathcal{T}_{\boldsymbol{I}} w) = \mathcal{T}_{\boldsymbol{I}} \boldsymbol{H}(w)$$
$$= \begin{cases} (-1)^r \boldsymbol{H}(w) & \text{if } \boldsymbol{H}(w) \text{ is an } r\text{th-order material tensor} \\ (-1)^{r+1} \boldsymbol{H}(w) & \text{if } \boldsymbol{H}(w) \text{ is an } r\text{th-order material pseudotensor.} \end{cases} \tag{4.64}$$

Hence $\boldsymbol{H}(w) = \boldsymbol{0}$ if it is an odd-order material tensor or an even-order pseudotensor. □

Figure 4.3: Data for left- and right-handed quartz

Table 6
Elasto-Piezo-Dielectric Matrices for Right- and Left-Handed Quartz

General form of the matrices

$$\left(\begin{array}{c|c} c^E & e_t \\ \hline e & \epsilon^S \end{array}\right)$$

c^E in 10^9 Pa

e in 10^{-2} C/m^2

ϵ^S in 10^{-12} F/m

Right-handed quartz

86.74	6.99	11.91	17.91	0	0	17.1	0	0
6.99	86.74	11.91	-17.91	0	0	-17.1	0	0
11.91	11.91	107.2	0	0	0	0	0	0
17.91	-17.91	0	57.94	0	0	4.06	4.06	0
0	0	0	0	57.94	35.82	0	0	0
0	0	0	0	35.82	39.88	0	-34.2	0
17.1	-17.1	0	4.06	0	0	39.21	0	0
0	0	0	4.06	0	-34.2	0	39.21	0
0	0	0	0	0	0	0	0	41.03

Left-handed quartz

86.74	6.99	11.91	17.91	0	0	-17.1	0	0
6.99	86.74	11.91	-17.91	0	0	17.1	0	0
11.91	11.91	107.2	0	0	0	0	0	0
17.91	-17.91	0	57.94	0	0	-4.06	-4.06	0
0	0	0	0	57.94	35.82	0	0	0
0	0	0	0	35.82	39.88	0	34.2	0
-17.1	17.1	0	-4.06	0	0	39.21	0	0
0	0	0	-4.06	0	34.2	0	39.21	0
0	0	0	0	0	0	0	0	41.03

NOTE: The matrix e_t is the transpose of the piezoelectric matrix e.

4.5 Treating Type II or III crystallites as if they are their Type I Laue-class peers: an equality of texture coefficients

In classical texture analysis, as the ODF is defined on SO(3), both G_{tex} and G_{cr} are subgroups of SO(3). When the theory of texture analysis is applied to a polycrystalline aggregate of crystallites whose G_{cr} is improper, it is routine practice to replace the improper G_{cr} by its peer proper group in the same Laue class. It is a puzzle that such an ad hoc procedure seemed to have often worked, and it is an objective of the present study to resolve this puzzle at least as far as material tensors and pseudotensors of weakly-textured polycrystals are concerned. Our answer will be based in part on a relation between the texture coefficients of a polycrystal with its G_{cr} being improper and its counterparts if the improper G_{cr} is replaced by its proper peer in the same Laue class. We will derive this relation in this section.

We may restrict our attention to the Laue classes which include Type I, Type II, and Type III crystals in the same class, as the discussions for the remaining cases (Laue classes 1, 3, and 10 in Table 2.2) are similar. The generic structures of the groups G_1, G_2, and G_3 in one such Laue class, which are of Type I, II, and III, respectively, are given in Section 4.2.1. We begin by considering a single crystal whose orientation with respect to the chosen reference is specified by rotation $\boldsymbol{R}_0$.

Suppose for the given single crystal $G_{\text{cr}} = G_1$. Then its orientation measure $\wp_1$ is given by (4.16), which we repeat below for convenience:

$$\wp_1 = \frac{1}{2N} \sum_{i=1}^{2N} \delta_{\boldsymbol{R}_0 \boldsymbol{R}_i}.$$

By the series expansion (4.3), the orthogonality relation (4.5), and the formula for $\wp_1$

above, we obtain [21]

$$
\begin{aligned}
c^l_{mn} &= \frac{2l+1}{8\pi^2} \int_{\mathrm{SO}(3)} \overline{D^l_{mn}(\boldsymbol{R})}\, d\wp_1 \\
&= \frac{2l+1}{8\pi^2} \int_{\mathrm{SO}(3)} \overline{D^l_{mn}(\boldsymbol{R})}\, d\left(\frac{1}{2N} \sum_{i=1}^{2N} \delta_{\boldsymbol{R}_0 \boldsymbol{R}_i} \right) \\
&= \frac{2l+1}{8\pi^2} \cdot \frac{1}{2N} \cdot \sum_{i=1}^{2N} \overline{D^l_{mn}(\boldsymbol{R}_0 \boldsymbol{R}_i)}. \qquad (4.65)
\end{aligned}
$$

Suppose the single crystal in question is of Type II and it has $G_{\mathrm{cr}} = G_2$. Then its orientation measure is given by (4.17), i.e.,

$$
\wp_2 = \frac{1}{4N} \left(\sum_{i=1}^{2N} \delta_{\boldsymbol{R}_0 \boldsymbol{R}_i} + \sum_{i=1}^{2N} \delta_{\boldsymbol{I} \boldsymbol{R}_0 \boldsymbol{R}_i} \right).
$$

By a similar argument as above but using the series expansion (4.56), we get

$$
\begin{aligned}
c^{l,R}_{mn} &= \frac{2l+1}{8\pi^2} \int_{\mathrm{SO}(3)} \overline{D^l_{mn}(\boldsymbol{R})}\, d\wp_2 \\
&= \frac{2l+1}{8\pi^2} \int_{\mathrm{SO}(3)} \overline{D^l_{mn}(\boldsymbol{R})}\, d\left(\frac{1}{4N} \sum_{i=1}^{2N} \delta_{\boldsymbol{R}_0 \boldsymbol{R}_i} \right) \\
&= \frac{2l+1}{8\pi^2} \cdot \frac{1}{4N} \cdot \sum_{i=1}^{2N} \overline{D^l_{mn}(\boldsymbol{R}_0 \boldsymbol{R}_i)}. \qquad (4.66)
\end{aligned}
$$

Similarly, we have

$$
c^{l,L}_{mn} = \frac{2l+1}{8\pi^2} \cdot \frac{1}{4N} \cdot \sum_{i=1}^{2N} \overline{D^l_{mn}(\boldsymbol{R}_0 \boldsymbol{R}_i)}. \qquad (4.67)
$$

If the single crystal is of Type III and has $G_{\mathrm{cr}} = G_2$, its orientation measure is given by (4.18), which reads

$$
\wp_3 = \frac{1}{2N} \left(\sum_{i=1}^{N} \delta_{\boldsymbol{R}_0 \boldsymbol{R}_i} + \sum_{i=N+1}^{2N} \delta_{\boldsymbol{I} \boldsymbol{R}_0 \boldsymbol{R}_i} \right).
$$

Using the series expansion (4.56) again, we obtain

$$\begin{aligned} c_{mn}^{l,R} &= \frac{2l+1}{8\pi^2}\int_{\mathrm{SO}(3)} \overline{D_{mn}^l(\boldsymbol{R})}\, d\wp_3 \\ &= \frac{2l+1}{8\pi^2}\int_{\mathrm{SO}(3)} \overline{D_{mn}^l(\boldsymbol{R})}\, d\left(\frac{1}{2N}\sum_{i=1}^{N}\delta_{\boldsymbol{R}_0\boldsymbol{R}_i}\right) \\ &= \frac{2l+1}{8\pi^2}\cdot\frac{1}{2N}\cdot\sum_{i=1}^{N}\overline{D_{mn}^l(\boldsymbol{R}_0\boldsymbol{R}_i)}. \end{aligned} \tag{4.68}$$

Similarly, we find

$$c_{mn}^{l,L} = \frac{2l+1}{8\pi^2}\cdot\frac{1}{2N}\cdot\sum_{i=N+1}^{2N}\overline{D_{mn}^l(\boldsymbol{R}_0\boldsymbol{R}_i)}. \tag{4.69}$$

Comparing equations (4.65) with (4.66) and (4.67), and with (4.68) and (4.69), we arrive at the following equation:

$$c_{mn}^{l}\ \text{(Type I)}\ =\ c_{mn}^{l,R} + c_{mn}^{l,L}\ \text{(Type II or III)}. \tag{4.70}$$

Clearly equation (4.70) remains valid for orientation measures defined by a finite number of orientations, where the texture coefficients in question are weighted averages (with volume fractions as weight) of the corresponding texture coefficients that pertain to each orientation.

In practice, a polycrystal is an aggregate of a finite number of crystallites with various orientations. In texture measurement by orientation imaging microscopy (OIM) using electron backscatter diffraction (EBSD), texture coefficients are computed, precisely by using (4.65), (4.66), (4.67), (4.68) and (4.69), from orientation measurements at a finite number of sampling points. Hence equality (4.70) is valid for all practical purposes in texture analysis.

On the other hand, for theoretical completeness the following question arises:

Does (4.70) hold not only for discrete measures but also for all corresponding ODFs (or absolutely-continuous orientation measures) pertaining to the two sides of the equation?

For aggregates of Type II crystallites, since $w^R = w^L = w_I/2$ (see Proposition (4.3.2); here w_I is the ODF on SO(3) that results if we replace $G_{\text{cr}} = G \cup \boldsymbol{I}G$ of the Type II crystallites by the rotational point group G in its Laue class), clearly (4.70) will always hold. For aggregates of Type III crystallites, according to Man [22] the answer to the question above is still affirmative.

We will henceforth use equality (4.70) freely in this thesis.

4.6 The extended representation theorem

The representation theorem of Man and Huang [20] concerns material tensors that pertain to weakly-textured aggregates of Type I crystallites. In this Section we extend their representation theorem to cover material tensors and pseudotensors that pertain to weakly-textured aggregates of Type II or Type III crystallites.

All orientation distribution functions w that pertain to polycrystalline aggregates of Type II or Type III crystallites satisfy the following two conditions:

1. When all texture coefficients $c^{l,+}_{00}$ and $c^{l,-}_{mn}$ with $l \geq 1$ are zero,

$$w(\boldsymbol{Q}) = w_{\text{iso}} = \frac{1}{16\pi^2} \qquad \text{for each } \boldsymbol{Q} \in \text{O}(3). \tag{4.71}$$

2.

$$\int_{\text{O}(3)} (w - w_{\text{iso}})\, d\mathcal{V} = 0. \tag{4.72}$$

Let

$$\mathcal{H}_0 = \{f \in L^2(\mathrm{O}(3)) : \int_{\mathrm{O}(3)} f\, d\mathcal{V} = 0\}, \tag{4.73}$$

$$\mathcal{H} = \{w \in L^2(\mathrm{O}(3)) : w = w_{\mathrm{iso}} + f, \text{ where } f \in \mathcal{H}_0\}. \tag{4.74}$$

For $r \geq 1$, let $Z \subset V^{\otimes r}$ be an invariant subspace of the tensor space $V^{\otimes r}$ under $\mathcal{T}_{\boldsymbol{Q}} = \boldsymbol{Q}^{\otimes r}$ (and, a fortiori, also under $\mathcal{T}_{\boldsymbol{Q}} = (\det \boldsymbol{Q})\, \boldsymbol{Q}^{\otimes r}$ for material pseudotensors) for each $\boldsymbol{Q} \in \mathrm{O}(3)$. Let $\mathcal{N}$ be an O(3)-invariant neighborhood of w_{iso} in $\mathcal{H}$ (i.e., if $w \in \mathcal{N}$, then $\mathcal{T}_{\boldsymbol{Q}} w \in \mathcal{N}$ for each $\boldsymbol{Q} \in \mathrm{O}(3)$). We consider material tensors (resp. pseudotensors) $\boldsymbol{H} : \mathcal{N} \to Z$ which are continuously differentiable in $\mathcal{N}$. Let $D\boldsymbol{H}(w_{\mathrm{iso}})[\cdot]$ denote the Fréchet derivative of $\boldsymbol{H}$ at w_{iso}.

Definition 4.6.1. *A polycrystalline aggegate of Type II or Type III crystallites is weakly-textured for the physical property characterized by the material tensor or pseudotensor* $\boldsymbol{H}$ *if, as far as the effect of texture on* $\boldsymbol{H}$ *is concerned, it is adequate to replace* $\boldsymbol{H}(w)$ *by its affine approximation at* w_{iso}*, i.e., we may put*

$$\boldsymbol{H}(w) = \boldsymbol{H}(w_{iso}) + D\boldsymbol{H}(w_{iso})[w - w_{iso}] + o(\|w - w_{iso}\|_{L^2}) \tag{4.75}$$

and ignore the $o(\|w - w_{iso}\|_{L^2})$ *term.*

Henceforth we shall restrict our attention to weakly-textured polycrystals.

By our basic assumption (4.60) and Proposition 4.3.3, we have

$$\mathcal{T}_{\boldsymbol{Q}} \boldsymbol{H}(w_{\mathrm{iso}}) = \boldsymbol{H}(\mathcal{T}_{\boldsymbol{Q}} w_{\mathrm{iso}}) = \boldsymbol{H}(w_{\mathrm{iso}}). \tag{4.76}$$

Hence the term $\boldsymbol{H}(w_{\mathrm{iso}})$ is an isotropic rth-order material tensor (reps. pseudotensor) in Z. The derivative $D\boldsymbol{H}(w_{\mathrm{iso}})[w - w_{\mathrm{iso}}]$ takes values in $Z \subset V^{\otimes r}$, and it is linear in the texture coefficients ($c_{mn}^{l,\pm}$ or $c_{mn}^{l,R/L}$). The following lemma follows easily from our basic assumption (4.60).

Lemma 4.6.2. *For each $\boldsymbol{Q} \in O(3)$ and each $w \in \mathcal{H}$,*

$$\mathcal{T}_{\boldsymbol{Q}}(D\boldsymbol{H}(w_{iso})[w - w_{iso}]) = D\boldsymbol{H}(w_{iso})[\mathcal{T}_{\boldsymbol{Q}}(w - w_{iso})]. \tag{4.77}$$

Proof. We start from the basic assumption $\mathcal{T}_{\boldsymbol{Q}}(\boldsymbol{H}(w)) = \boldsymbol{H}(\mathcal{T}_{\boldsymbol{Q}} w)$. On the left-hand side of the equation, we have

$$\mathcal{T}_{\boldsymbol{Q}}(\boldsymbol{H}(w)) = \mathcal{T}_{\boldsymbol{Q}}(\boldsymbol{H}(w_{\text{iso}}) + D\boldsymbol{H}(w_{\text{iso}})[w - w_{\text{iso}}] + o(\|w - w_{\text{iso}}\|_{L^2})). \tag{4.78}$$

On the right-hand side, we put $w = w_{\text{iso}} + (w - w_{\text{iso}})$ and get

$$\begin{aligned}\boldsymbol{H}(\mathcal{T}_{\boldsymbol{Q}} w) &= \boldsymbol{H}(\mathcal{T}_{\boldsymbol{Q}} w_{\text{iso}} + \mathcal{T}_{\boldsymbol{Q}}(w - w_{\text{iso}})) \\ &= \boldsymbol{H}(\mathcal{T}_{\boldsymbol{Q}} w_{\text{iso}}) + D\boldsymbol{H}(\mathcal{T}_{\boldsymbol{Q}} w_{\text{iso}})[\mathcal{T}_{\boldsymbol{Q}}(w - w_{\text{iso}})] + o(\|\mathcal{T}_{\boldsymbol{Q}}(w - w_{\text{iso}})\|_{L^2})). \end{aligned} \tag{4.79}$$

Equating (4.78) and (4.79), we obtain (4.77) because $\mathcal{T}_{\boldsymbol{Q}}(\boldsymbol{H}(w_\alpha)) = \boldsymbol{H}(\mathcal{T}_{\boldsymbol{Q}} w_\alpha)$, $\mathcal{T}_{\boldsymbol{Q}} w_{\text{iso}} = w_{\text{iso}}$, $\mathcal{T}_{\boldsymbol{Q}} : V^{\otimes r} \to V^{\otimes r}$ is unitary, and $\mathcal{T}_{\boldsymbol{Q}} : L^2(O(3)) \to L^2(O(3))$ ($w \mapsto \mathcal{T}_{\boldsymbol{Q}} w$) is norm-preserving. □

For material tensors that pertain to polycrystalline aggregates of Type I crystallites, Man and Huang [20] derived a representation theorem that delineates the explicit dependence of $D\boldsymbol{H}(w_{\text{iso}})[w - w_{\text{iso}}]$ on texture coefficients. Here we will follow their arguments and extend their theorem to cover aggregates of Type II or Type III crystallites.

Every subspace of rth-order tensors ($r = 0, 1, 2, \cdots$) invariant under $\boldsymbol{Q}^{\otimes r}$ can be written as a direct sum of irreducible invariant subspaces on each of which the representation $\boldsymbol{Q} \to \boldsymbol{Q}^{\otimes r}$ is equivalent to one of the irreducible unitary representations $\mathcal{D}_k^{\pm}$. To start with, we derive a representation theorem for material tensors (resp. pseudotensors) of weakly-textured polycrystals that satisfy condition (4.77) and belong to a specific irreducible invariant subspace.

Theorem 4.6.3. *For $k \geq 1$, let Z be a $(2k+1)$-dimensional subspace of $V^{\otimes r}$ invariant under $\boldsymbol{Q}^{\otimes r}$ for each $\boldsymbol{Q} \in \mathrm{O}(3)$, and let Z_c be its complexification. Let $\boldsymbol{H}_m$ $(-k \leq m \leq k)$ be an orthonormal irreducible tensor basis in Z_c, which satisfies $\boldsymbol{H}_m = (-1)^m \overline{\boldsymbol{H}_{\bar{m}}}$.*[②] *Let $\boldsymbol{H} : \mathcal{H} \to Z_c$ be a material tensor (resp. pseudotensor) that pertains to a polycrystalline aggregate of Type II or Type III crystallites, and let $\boldsymbol{H}$ be differentiable at w_{iso}. Suppose the restriction of the representation $\boldsymbol{Q} \mapsto \mathcal{T}_{\boldsymbol{Q}}$ on Z_c, where $\mathcal{T}_{\boldsymbol{Q}} = \boldsymbol{Q}^{\otimes r}$ for material tensor and $\mathcal{T}_{\boldsymbol{Q}} = (\det \boldsymbol{Q})\,\boldsymbol{Q}^{\otimes r}$ for material pseudotensor, is equivalent to the irreducible unitary representation $\mathcal{D}_k^+$ when r is even for material tensor (resp. odd for pseudotensor) or to $\mathcal{D}_k^-$ when r is odd for material tensor (resp. even for pseudotensor). Let $D\boldsymbol{H}(w_{iso}) : \mathcal{H}_0 \to Z$, the Frechét derivative of $\boldsymbol{H}$ at w_{iso}, satisfy condition (4.77) for each $\boldsymbol{Q} \in \mathrm{O}(3)$ and for each $w - w_{\mathrm{iso}} \in \mathcal{H}_0$. When r is even for material tensor (resp. odd for pseudotensor), we have:*

$$D\boldsymbol{H}(w_{\mathrm{iso}})[w - w_{\mathrm{iso}}] = \sum_{n,m=-k}^{k} \alpha_n^k (c_{mn}^{k,R} + c_{mn}^{k,L}) \boldsymbol{H}_m; \tag{4.80}$$

when r is odd for material tensor (resp. even for pseudotensor), there holds:

$$D\boldsymbol{H}(w_{\mathrm{iso}})[w - w_{\mathrm{iso}}] = \sum_{n,m=-k}^{k} \alpha_n^k (c_{mn}^{k,R} - c_{mn}^{k,L}) \boldsymbol{H}_m; \tag{4.81}$$

here $c_{mn}^{k,R}$ and $c_{mn}^{k,L}$ are texture coefficients that pertain to w^R and w^L, respectively, and $\alpha_n^{k,s}$ are (complex) undetermined parameters. The parameters α_n^k satisfy:

$$\alpha_n^k = (-1)^n \overline{\alpha_{\bar{n}}^k}. \tag{4.82}$$

Proof. Let $\mathcal{H}_0^c$ be the complexification of $\mathcal{H}_0$. We extend the function $D\boldsymbol{H} : \mathcal{H}_0 \to Z$ to a linear mapping from $\mathcal{H}_0^c$ to Z_c, which we still denote by $D\boldsymbol{H}$, defined by

$$D\boldsymbol{H}[f + \sqrt{-1}h] = D\boldsymbol{H}[f] + \sqrt{-1} D\boldsymbol{H}[h] \tag{4.83}$$

for each $f, h \in \mathcal{H}_0$. Condition (4.77) remains valid after this extension.

Man and Huang [20] showed the existence of the orthonormal tensors $\boldsymbol{H}_m^k$ and provided a procedure for their construction. Let us proceed to consider formula (4.80) for even-

[②] Cf. [20] for the existence and a procedure for the construction of such a basis.

order material tensors and odd-order pseudotensors. Since the tensors $\boldsymbol{H}_m$ $(-k \le m \le k)$ constitute a basis in Z_c, we may write

$$D\boldsymbol{H}(w_{\text{iso}})[w - w_{\text{iso}}] = \sum_{p=-k}^{k} \beta_p(w_{\text{iso}})[w - w_{\text{iso}}]\boldsymbol{H}_p, \tag{4.84}$$

for some linear functioals $\beta_p : \mathcal{H}_0 \to \mathbb{C}$. As the domain of $D\boldsymbol{H}$ is extended to $\mathcal{H}_0^c$ according to (4.83), the linear functions β_p are likewise extended accordingly. By (4.77) and (4.84), we have

$$\begin{aligned}\mathcal{T}_{\boldsymbol{Q}}(D\boldsymbol{H}(w_{\text{iso}})[w - w_{\text{iso}}]) &= D\boldsymbol{H}(\mathcal{T}_{\boldsymbol{Q}} w_{\text{iso}})[\mathcal{T}_{\boldsymbol{Q}}(w - w_{\text{iso}})] \\ &= \sum_{p=-k}^{k} \beta_p(\mathcal{T}_{\boldsymbol{Q}} w_{\text{iso}})[\mathcal{T}_{\boldsymbol{Q}}(w - w_{\text{iso}})]\boldsymbol{H}_p \\ &= \sum_{p=-k}^{k} \beta_p(w_{\text{iso}})[\mathcal{T}_{\boldsymbol{Q}} w - \mathcal{T}_{\boldsymbol{Q}} w_{\text{iso}}]\boldsymbol{H}_p. \end{aligned} \tag{4.85}$$

for each $w - w_{\text{iso}}$ in $\mathcal{H}_0^c$. (Notice that here $\mathcal{T}_{\boldsymbol{Q}}$ has two different meanings which should be clear from the context.) Substituting

$$\begin{aligned}\mathcal{T}_{\boldsymbol{Q}} w(\boldsymbol{Q}_1) - \mathcal{T}_{\boldsymbol{Q}} w_{\text{iso}} &= \sum_{l=1}^{\infty}\sum_{m=-l}^{l}\sum_{n=-l}^{l} c_{mn}^{l,+} D_{mn}^{l,+}(\boldsymbol{Q}^T\boldsymbol{Q}_1) + \sum_{l=1}^{\infty}\sum_{m=-l}^{l}\sum_{n=-l}^{l} c_{mn}^{l,-} D_{mn}^{l,-}(\boldsymbol{Q}^T\boldsymbol{Q}_1) \\ &= \sum_{l=1}^{\infty}\sum_{m=-l}^{l}\sum_{n=-l}^{l} c_{mn}^{l,+}\left(\sum_{s=-l}^{l} D_{ms}^{l,+}(\boldsymbol{Q}^T) D_{sn}^{l,+}(\boldsymbol{Q}_1)\right) \\ &+ \sum_{l=1}^{\infty}\sum_{m=-l}^{l}\sum_{n=-l}^{l} c_{mn}^{l,-}\left(\sum_{s=-l}^{l} D_{ms}^{l,-}(\boldsymbol{Q}^T) D_{sn}^{l,-}(\boldsymbol{Q}_1)\right)\end{aligned} \tag{4.86}$$

into equation (4.85) and multiplying both sides of the equation on the left by $\mathcal{T}_{\boldsymbol{Q}^T}$, we obtain

$$
\begin{aligned}
D\boldsymbol{H}(w_{\text{iso}})[w - w_{\text{iso}}] &= \sum_{l=1}^{\infty} \sum_{m,n,s=-l}^{l} \sum_{p=-k}^{k} c_{mn}^{l,+} \beta_p [D_{sn}^{l,+}(\cdot)] D_{ms}^{l,+}(\boldsymbol{Q}^T) \left(\mathcal{T}_{\boldsymbol{Q}^T} \boldsymbol{H}_p \right) \\
&+ \sum_{l=1}^{\infty} \sum_{m,n,s=-l}^{l} \sum_{p=-k}^{k} c_{mn}^{l,-} \beta_p (w_{\text{iso}}) [D_{sn}^{l,-}(\cdot)] D_{ms}^{l,-}(\boldsymbol{Q}^T) \left(\mathcal{T}_{\boldsymbol{Q}^T} \boldsymbol{H}_p \right) \\
&= \sum_{l=1}^{\infty} \sum_{m,n,s=-l}^{l} \sum_{p=-k}^{k} c_{mn}^{l,+} \beta_p (w_{\text{iso}}) [D_{sn}^{l,+}(\cdot)] D_{ms}^{l,+}(\boldsymbol{Q}^T) \left(\sum_{q=-k}^{k} D_{pq}^{k,+}(\boldsymbol{Q}) \boldsymbol{H}_q \right) \\
&+ \sum_{l=1}^{\infty} \sum_{m,n,s=-l}^{l} \sum_{p=-k}^{k} c_{mn}^{l,-} \beta_p (w_{\text{iso}}) [D_{sn}^{l,-}(\cdot)] D_{ms}^{l,-}(\boldsymbol{Q}^T) \left(\sum_{q=-k}^{k} D_{pq}^{k,+}(\boldsymbol{Q}) \boldsymbol{H}_q \right) \\
&= \sum_{l=1}^{\infty} \sum_{m,n,s=-l}^{l} \sum_{p,q=-k}^{k} c_{mn}^{l,+} \beta_p (w_{\text{iso}}) [D_{sn}^{l,+}(\cdot)] \overline{D_{sm}^{l,+}(\boldsymbol{Q})} D_{pq}^{k,+}(\boldsymbol{Q}) \boldsymbol{H}_q \\
&+ \sum_{l=1}^{\infty} \sum_{m,n,s=-l}^{l} \sum_{p,q=-k}^{k} c_{mn}^{l,-} \beta_p (w_{\text{iso}}) [D_{sn}^{l,-}(\cdot)] \overline{D_{sm}^{l,-}(\boldsymbol{Q})} D_{pq}^{k,+}(\boldsymbol{Q}) \boldsymbol{H}_q, \qquad (4.87)
\end{aligned}
$$

where we have appealed to $\mathcal{T}_{\boldsymbol{Q}} \boldsymbol{H}_m = \sum_{p=-k}^{k} D_{mp}^{k,+}(\boldsymbol{Q}^T) \boldsymbol{H}_p$ as in Corollary 3.3.2 and to the properties of the Wigner D-functions. Integrating both sides of the preceding equation over the orthogonal group with respect to $\boldsymbol{Q}$, we derive from the orthogonal relation (cf. (3.14), (3.15) and (3.17)) that

$$
\begin{aligned}
D\boldsymbol{H}(w_{\text{iso}})[w - w_{\text{iso}}] &= \int_{\mathrm{O}(3)} D\boldsymbol{H}(w_{\text{iso}})[w - w_{\text{iso}}] dg \\
&= \sum_{l=1}^{\infty} \sum_{m,n,s=-l}^{l} \sum_{p,q=-k}^{k} c_{mn}^{l,+} \beta_p (w_{\text{iso}}) [D_{sn}^{l,+}(\cdot)] \left(\int_{\mathrm{O}(3)} \overline{D_{sm}^{l,+}(\boldsymbol{Q})} D_{pq}^{k,+}(\boldsymbol{Q}) dg \right) \boldsymbol{H}_q \\
&+ \sum_{l=1}^{\infty} \sum_{m,n,s=-l}^{l} \sum_{p,q=-k}^{k} c_{mn}^{l,-} \beta_p (w_{\text{iso}}) [D_{sn}^{l,-}(\cdot)] \left(\int_{\mathrm{O}(3)} \overline{D_{sm}^{l,-}(\boldsymbol{Q})} D_{pq}^{k,+}(\boldsymbol{Q}) dg \right) \boldsymbol{H}_q \\
&= \sum_{l=1}^{\infty} \sum_{m,n,s=-l}^{l} \sum_{p,q=-k}^{k} c_{mn}^{l,+} \beta_p (w_{\text{iso}}) [D_{sn}^{l,+}(\cdot)] \left(\frac{1}{2k+1} \delta_{lk} \delta_{sp} \delta_{mq} \right) \boldsymbol{H}_q \\
&= \frac{1}{2k+1} \sum_{n=-k}^{k} \sum_{p=-k}^{k} \sum_{m=-k}^{k} c_{mn}^{k,+} \beta_p (w_{\text{iso}}) [D_{pn}^{k,+}(\cdot)] \boldsymbol{H}_m \\
&= \sum_{n=-k}^{k} \tilde{\alpha}_n^k \left(\sum_{m=-k}^{k} c_{mn}^{k,+} \boldsymbol{H}_m \right) \\
&= \sum_{n=-k}^{k} \alpha_n^k \left(\sum_{m=-k}^{k} (c_{mn}^{k,R} + c_{mn}^{k,L}) \boldsymbol{H}_m \right), \qquad (4.88)
\end{aligned}
$$

where last equality follows from $(4.47)_1$ and

$$\alpha_n^k = \frac{1}{2}\tilde{\alpha}_n^k = \frac{1}{4k+2}\sum_{p=-k}^{k}\beta_p(w_{\text{iso}})[D_{pn}^{k,+}(\cdot)]. \tag{4.89}$$

Next we proceed to prove (4.81). For odd-order material tensors and even-order pseudotensors, we have $\mathcal{T}_{\boldsymbol{Q}}\boldsymbol{H}_m = \sum_{p=-k}^{k} D_{mp}^{k,-}(\boldsymbol{Q}^T)\boldsymbol{H}_p$ as in Corollary 3.3.2. Instead of (4.87), we have

$$\begin{aligned} D\boldsymbol{H}(w_{\text{iso}})[w - w_{\text{iso}}] = &\sum_{l=1}^{\infty}\sum_{m,n,s=-l}^{l}\sum_{p,q=-k}^{k} c_{mn}^{l,+}\beta_p(w_{\text{iso}})[D_{sn}^{l,+}(\cdot)]\overline{D_{sm}^{l,+}(\boldsymbol{Q})}D_{pq}^{k,-}(\boldsymbol{Q})\boldsymbol{H}_q \\ &+\sum_{l=1}^{\infty}\sum_{m,n,s=-l}^{l}\sum_{p,q=-k}^{k} c_{mn}^{l,-}\beta_p(w_{\text{iso}})[D_{sn}^{l,-}(\cdot)]\overline{D_{sm}^{l,-}(\boldsymbol{Q})}D_{pq}^{k,-}(\boldsymbol{Q})\boldsymbol{H}_q. \end{aligned} \tag{4.90}$$

And then (4.88) is replaced by:

$$\begin{aligned} D\boldsymbol{H}(w_{\text{iso}})[w - w_{\text{iso}}] &= \int_{\mathrm{O}(3)} D\boldsymbol{H}(w_{\text{iso}})[w - w_{\text{iso}}]dg \\ &= \sum_{l=1}^{\infty}\sum_{m,n,s=-l}^{l}\sum_{p,q=-k}^{k} c_{mn}^{l,+}\beta_p(w_{\text{iso}})[D_{sn}^{l,+}(\cdot)]\left(\int_{\mathrm{O}(3)}\overline{D_{sm}^{l,+}(\boldsymbol{Q})}D_{pq}^{k,-}(\boldsymbol{Q})dg\right)\boldsymbol{H}_q \\ &+\sum_{l=1}^{\infty}\sum_{m,n,s=-l}^{l}\sum_{p,q=-k}^{k} c_{mn}^{l,-}\beta_p(w_{\text{iso}})[D_{sn}^{l,-}(\cdot)]\left(\int_{\mathrm{O}(3)}\overline{D_{sm}^{l,-}(\boldsymbol{Q})}D_{pq}^{k,-}(\boldsymbol{Q})dg\right)\boldsymbol{H}_q \\ &= \sum_{l=1}^{\infty}\sum_{m,n,s=-l}^{l}\sum_{p,q=-k}^{k} c_{mn}^{l,-}\beta_p(w_{\text{iso}})[D_{sn}^{l,-}(\cdot)]\left(\frac{1}{2k+1}\delta_{lk}\delta_{sp}\delta_{mq}\right)\boldsymbol{H}_q \\ &= \frac{1}{2k+1}\sum_{n=-k}^{k}\sum_{p=-k}^{k}\sum_{m=-k}^{k} c_{mn}^{k,-}\beta_p(w_{\text{iso}})[D_{pn}^{k,-}(\cdot)]\boldsymbol{H}_m \\ &= \sum_{n=-k}^{k}\tilde{\alpha}_n^k\left(\sum_{m=-k}^{k} c_{mn}^{k,-}\boldsymbol{H}_m\right) \\ &= \sum_{n=-k}^{k}\alpha_n^k\left(\sum_{m=-k}^{k}(c_{mn}^{k,R} - c_{mn}^{k,L})\boldsymbol{H}_m\right) \end{aligned} \tag{4.91}$$

where the last equality follows from $(4.47)_2$ and

$$\alpha_n^k = \frac{1}{2}\tilde{\alpha}_n^k = \frac{1}{4k+2}\sum_{p=-k}^{k}\beta_p(w_{\text{iso}})[D_{pn}^{k,-}(\cdot)]. \tag{4.92}$$

Finally the properties in (4.82) on the (complex) undetermined parameters α_n^k can be derived by the fact that $w - w_{\text{iso}} \in \mathcal{H}_0$ is real-valued, i.e., $\boldsymbol{DH}[w - w_{\text{iso}}] \in Z$ and thus $\overline{\boldsymbol{DH}[w - w_{\text{iso}}]} = \boldsymbol{DH}[w - w_{\text{iso}}]$. We refer the reader for the proof in Man and Huang's work [20]. □

Theorem 3.3.3 shows the decomposition formula for the tensor and pseudotensor representations of the orthogonal group. Applying Theorem 4.6.3 to each of the irreducible invariant subspaces of Z_c in the decomposition formula, we have the following representation theorem for material tensors and pseudotensors that pertain to weakly-textured aggregates of Type II or Type III crystallites.

Theorem 4.6.4. *Let $Z \subset V^{\otimes r}$ be a tensor (resp. pseudotensor) space invariant under the action of the orthogonal group. Let $\boldsymbol{H}(w) \in Z$ be a material tensor (resp. pseudotensor) pertaining to a weakly-textured polycrystal of Type II or Type III crystallites. Let equation (3.31) be the decomposition of Z_c, the complexification of Z, into its irreducible parts under O(3). For each k in $J := \{j : n_j \neq 0\}$ and $1 \leq s \leq n_k$, there exists a family of orthonormal irreducible basis tensors $\boldsymbol{H}_m^{k,s} \in Z_c$ $(-k \leq m \leq k)$ for which the following representation formula is valid when r is even (resp. odd):*

$$\boldsymbol{H}(w) = \sum_{k \in J} \sum_{s=1}^{n_k} \sum_{m,n=-k}^{k} \alpha_n^{k,s} (c_{mn}^{k,R} + c_{mn}^{k,L}) \boldsymbol{H}_m^{k,s}. \tag{4.93}$$

When r is odd (resp. even), the formula is:

$$\boldsymbol{H}(w) = \sum_{k \in J} \sum_{s=1}^{n_k} \sum_{m,n=-k}^{k} \alpha_n^{k,s} (c_{mn}^{k,R} - c_{mn}^{k,L}) \boldsymbol{H}_m^{k,s}. \tag{4.94}$$

where $c_{mn}^{k,R/L}$ are texture coefficients[③] *of w^R and w^L, respectively, and $\alpha_n^{k,s}$ are (complex) undetermined parameters. For each $k \in J$ and $1 \leq s \leq n_k$, the orthonormal tensors $\boldsymbol{H}_m^{k,s}$ and parameters $\alpha_n^{k,s}$ enjoy the following properties (see also Corollary (3.3.2)):*

$$\boldsymbol{H}_m^{k,s} = (-1)^m \overline{\boldsymbol{H}_{\bar{m}}^{k,s}}, \qquad \alpha_n^{k,s} = (-1)^n \overline{\alpha_{\bar{n}}^{k,s}}. \tag{4.95}$$

[③] $c_{00}^{0,R/L} := 1/(16\pi^2)$

In summary, the following representation formula holds for material tensors and pseudotensors $\boldsymbol{H}(w)$ of weakly-textured polycrystals:

$$\boldsymbol{H}(w) = \sum_{l\in J} \sum_{s=1}^{n_l} \sum_{m,n=-l}^{l} \alpha_n^{l,s} b_{mn}^l \boldsymbol{H}_m^{l,s}, \tag{4.96}$$

where $\alpha_n^{l,s}$ are undetermined material parameters and b_{mn}^l are given by the texture coefficients as follows:

1. For aggregates of Type I crystallites, we have $b_{mn}^l = c_{mn}^l$ (see Man and Huang [20]).

2. For aggregates of Type II or Type III crystallites, we have

$$b_{mn}^l = \begin{cases} c_{mn}^{l,R} + c_{mn}^{l,L} = c_{mn}^l, & \text{for even order [r] and odd order [p]} \\ c_{mn}^{l,R} - c_{mn}^{l,L} \neq c_{mn}^l, & \text{for odd order [r] and even order [p];} \end{cases} \tag{4.97}$$

   here [r] denotes (regular) material tensors and [p] denotes material pesudotensors, and c_{mn}^l are the texture coefficients of the ODF in classical texture analysis, where Type II and Type III crystallites are treated as if they are their Type I Laue-class peers.

Remark: Work in classical texture analysis was concentrated on fcc, bcc, and hcp metals, with G_{cr} in question being the Type II O_h (fcc, bcc) and D_{6h} (hcp). For aggregates of Type II crystallites, we have $w^R = w^L = w_I/2$ (see Proposition 4.3.2), where w_I is the ODF of the polycrystal when the Type II crystallites with $G_{\text{cr}} = G \cup \boldsymbol{I}G$, where G is of Type I, are treated as if their $G_{\text{cr}} = G$ (e.g. crystallites with $G_{\text{cf}} = O_h$ are treated as if their group of crystal symmetry is O). The material properties studied in classical texture analysis were those involving even-order material tensors, because all odd-order material tensors of Type II aggregates are zero (see Proposition 4.4.1). For even-order material tensors of weakly-textured polycrystals, by the representation formula (4.93) and the equality (4.70) on texture coefficients, we see that no error will be made by treating crystallites with $G_{cr} = O_h$ (resp. D_{6h}) as if their $G_{cr} = O$ (resp. D_6). In particular, X-ray diffraction (modulo its other limitations) may be used to determine the texture coefficients in question.

Remark: For aggregates of Type III crystallites, X-ray diffraction (XRD) can determine only sums of texture coefficients of the form $c^{l,R}_{mn} + c^{l,L}_{mn}$. To determine odd-order material tensors and even-order pseudotensors of weakly-textured Type III polycrystals, however, by representation formula (4.94) we should ascertain the differences $c^{l,R}_{mn} - c^{l,L}_{mn}$. XRD alone cannot provide the required information.

4.7 An alternate proof the extended representation theorem

Let $f_{\text{iso}} := 1/(8\pi^2)$ and $\lambda \in [0,1]$. We consider aggregate mixtures of right- and left-handed crystallites with volume fractions λ and $1-\lambda$, respectively. Let

$$\mathcal{H}_0 := \{h \in L^2(\mathrm{SO}(3)) : \int_{\mathrm{SO}(3)} h\, dg = 0\}, \tag{4.98}$$

$$\mathcal{H} := \{f \in L^2(\mathrm{SO}(3)) : f = f_{\text{iso}} + h, \text{ where } h \in \mathcal{H}_0\}. \tag{4.99}$$

Let Z be a space of rth-order tensors. We assume that

$$\boldsymbol{H} : \mathcal{H} \times \mathcal{H} \times [0,1] \to Z, \quad (f^R, f^L, \lambda) \mapsto \boldsymbol{H}(f^R, f^L, \lambda), \tag{4.100}$$

where λ stands for the volume fraction of right-handed crystallites, is continuously differentiable. For a given λ, the restriction $\boldsymbol{H}(\cdot,\cdot,\lambda)$ can be written as

$$\boldsymbol{H}_\lambda : \lambda\mathcal{H} \times (1-\lambda)\mathcal{H} \to Z, \quad (w^R, w^L) \mapsto \boldsymbol{H}_\lambda(w^R, w^L), \tag{4.101}$$

where

$$\mu\mathcal{H} := \{\mu f : f \in \mathcal{H}\} \text{ for any } \mu \in [0,1], \quad w^R = \lambda f^R, \quad w^L = (1-\lambda) f^L. \tag{4.102}$$

One consequence of our basic physical assumption (4.60) is that

$$\boldsymbol{H}_\lambda(w^R, w^L) = \begin{cases} \boldsymbol{H}_{(1-\lambda)}(\tilde{w}^R, \tilde{w}^L), & \text{for even order [r] and odd order [p]} \\ -\boldsymbol{H}_{(1-\lambda)}(\tilde{w}^R, \tilde{w}^L), & \text{for odd order [r] and even order [p],} \end{cases} \tag{4.103}$$

where $\tilde{w}^R = w^L = \frac{1}{2}f^L, \tilde{w}^L = w^R = \frac{1}{2}f^R$, for any $f^R, f^L \in \mathcal{H}$; here [r] denotes (regular) material tensors and [p] denotes material pesudotensors. When $\lambda = \frac{1}{2}$, we shall suppress the subscript in $\boldsymbol{H}_{\frac{1}{2}}(w^R, w^L)$ and simply write $\boldsymbol{H}(w^R, w^L)$. In this case, the above equation reads

$$\boldsymbol{H}(w^R, w^L) = \begin{cases} \boldsymbol{H}(w^L, w^R), & \text{for even order [r] and odd order [p]} \\ -\boldsymbol{H}(w^L, w^R), & \text{for odd order [r] and even order [p]} \end{cases} \tag{4.104}$$

for any $w^R, w^L \in \frac{1}{2}\mathcal{H}$.

Lemma 4.7.1. *Let $w_o = \frac{1}{2}f_{iso} = 1/(16\pi^2)$. Then we have*

$$\begin{aligned} &D_1\boldsymbol{H}(w_o, w_o)[w - w_o] \\ &= \begin{cases} D_2\boldsymbol{H}(w_o, w_o)[w - w_o], & \text{for even order [r] and odd order [p]} \\ -D_2\boldsymbol{H}(w_o, w_o)[w - w_o], & \text{for odd order [r] and even order [p]} \end{cases} \end{aligned} \tag{4.105}$$

for each $w \in \frac{1}{2}\mathcal{H}$.

Proof. Let us first consider material tensors of even order and pseudotensors of odd order. For each $w \in \frac{1}{2}\mathcal{H}$, we have

$$\boldsymbol{H}(w, w_o) = \boldsymbol{H}(w_o, w_o) + D_1\boldsymbol{H}(w_o, w_o)[w - w_o] + o(\|w - w_o\|), \tag{4.106}$$

and

$$\boldsymbol{H}(w_o, w) = \boldsymbol{H}(w_o, w_o) + D_2\boldsymbol{H}(w_o, w_o)[w - w_o] + o(\|w - w_o\|). \tag{4.107}$$

Since by (4.104) we have $\boldsymbol{H}(w, w_o) = \boldsymbol{H}(w_o, w)$ for each $w \in \frac{1}{2}\mathcal{H}$, the conclusion follows. For material tensors of odd order and pseudotensors of even order, we have $\boldsymbol{H}(w, w_o) = -\boldsymbol{H}(w_o, w)$. It follows that $\boldsymbol{H}(w_o, w_o) = -\boldsymbol{H}(w_o, w_o)$, and we observe that $\boldsymbol{H}(w_o, w_o) = \boldsymbol{0}$. The conclusion then follows from (4.104), (4.106), and (4.107). □

Now let us start by restricting our attention to material tensors of even order and pseudotensors of odd order. Let

$$f^R(\boldsymbol{R}) = \sum_{k=0}^{\infty} \sum_{m,n=-k}^{k} c_{mn}^{k,R} D_{mn}^k(\boldsymbol{R}), \quad f^L(\boldsymbol{R}) = \sum_{k=0}^{\infty} \sum_{m,n=-k}^{k} c_{mn}^{k,L} D_{mn}^k(\boldsymbol{R}) \tag{4.108}$$

be the expansions of f^R and f^L in terms of the Wigner D-functions.

It follows from Lemma 4.7.1 and the representation formula of Man and Huang [20] that for weakly-textured polycrystalline aggregates of Type II or Type III crystallites we have

$$\begin{aligned}
\boldsymbol{H}(w^R, w^L) &\simeq \boldsymbol{H}(w_o, w_o) + D_1\boldsymbol{H}(w_o, w_o)[w^R - w_o] + D_2\boldsymbol{H}(w_o, w_o)[w^L - w_o] \\
&= \boldsymbol{H}(w_o, w_o) + \sum_{l\neq 0, l\in J} \sum_{s=1}^{n_l} \sum_{m,n=-l}^{l} \alpha_n^{l,s} c_{mn}^{l,R} \boldsymbol{H}_m^{l,s} + \sum_{l\neq 0, l\in J} \sum_{s=1}^{n_l} \sum_{m,n=-l}^{l} \alpha_n^{l,s} c_{mn}^{l,L} \boldsymbol{H}_m^{l,s} \\
&= \boldsymbol{H}(w_o, w_o) + \sum_{l\neq 0, l\in J} \sum_{s=1}^{n_l} \sum_{m,n=-l}^{l} \alpha_n^{l,s} \left(c_{mn}^{l,R} + c_{mn}^{l,L}\right) \boldsymbol{H}_m^{l,s} \\
&= \boldsymbol{H}(w_o, w_o) + \sum_{l\neq 0, l\in J} \sum_{s=1}^{n_l} \sum_{m,n=-l}^{l} \alpha_n^{l,s} b_{mn}^{l} \boldsymbol{H}_m^{l,s}. \qquad (4.109)
\end{aligned}$$

where $\alpha_n^{l,s}$ are undetermined materials parameters and $b_{mn}^l = c_{mn}^{l,R} + c_{mn}^{l,L}$.

Similarly, for tensors of odd order and pseudotensors of even order that pertain to weakly-textured polycrystals of Type II or Type III crystallites, we have

$$\begin{aligned}
\boldsymbol{H}(w^R, w^L) &\simeq \sum_{l\neq 0, l\in J} \sum_{s=1}^{n_l} \sum_{m,n=-l}^{l} \alpha_n^{l,s} \left(c_{mn}^{l,R} - c_{mn}^{l,L}\right) \boldsymbol{H}_m^{l,s} \\
&= \sum_{l\neq 0, l\in J} \sum_{s=1}^{n_l} \sum_{m,n=-l}^{l} \alpha_n^{l,s} b_{mn}^{l} \boldsymbol{H}_m^{l,s}. \qquad (4.110)
\end{aligned}$$

where $b_{mn}^l = c_{mn}^{l,R} - c_{mn}^{l,L}$.

Finally let us summarize by including the information given by Man and Huang [20] on weakly-textured polycrystals of Type I crystallites. For even-order material tensors and odd-order pseudotensors of weakly-textured polycrystals , we have

$$\boldsymbol{H}(w) = \sum_{l\in J} \sum_{s=1}^{n_l} \sum_{m,n=-l}^{l} \alpha_n^{l,s} b_{mn}^{l} \boldsymbol{H}_m^{l,s}, \qquad (4.111)$$

where

$$b_{mn}^l = c_{mn}^l \ \text{(Type I)}, \quad b_{mn}^l = c_{mn}^{R,l} + c_{mn}^{L,l} \ \text{(Types II and III)} \qquad (4.112)$$

For odd-order material tensors of and even-order pseudotensors of weakly-textured polycrystals, similarly we have

$$\boldsymbol{H}(w) = \sum_{l\in J} \sum_{s=1}^{n_l} \sum_{m,n=-l}^{l} \alpha_n^{l,s} b_{mn}^{l} \boldsymbol{H}_m^{l,s}, \tag{4.113}$$

where

$$b_{mn}^{l} = c_{mn}^{l} \ \text{(Type I)}, \quad b_{mn}^{l} = 0 \ \text{(Type II)}, \quad b_{mn}^{l} = c_{mn}^{R,l} - c_{mn}^{L,l} \ \text{(Type III)}. \tag{4.114}$$

For aggregates of crystallites with G_{cr} in the same Laue class (e.g., O, O_h, T_d), by (4.70) the equality $c_{mn}^{l} = c_{mn}^{R,l} + c_{mn}^{L,l}$ is always valid.

Remark: The shorter alternate proof of the extended representation theorem given in this section is heavily based on the theorem of Man and Huang [20]. The much longer arguments that lead to Theorems 4.6.3 and 4.6.4 in the preceding section follow the same lines as in Man and Huang's proof of their theorem and can be regarded as a generalized version of their proof. In fact the proof of Man and Huang's representation theorem and that of Theorem 4.6.4 can be easily combined to become the proof of one theorem that covers material tensors and pseudotensors of weakly textured polycrystals with G_{cr} being any crystallographic point group.

Chapter 5 Restrictions on texture coefficients

5.1 Transformation formulas

5.1.1 Crystal symmetry

When the reference crystal lattice of the crystallites undergoes a rotation or roto-inversion defined by $\boldsymbol{Q}_2 \in \mathrm{O}(3)$, the ODF of the polycrystal becomes $\tilde{w}$, which is related to the original ODF w by $\tilde{w}(\boldsymbol{Q}_1) = w(\boldsymbol{Q}_1\boldsymbol{Q}_2)$ for each $\boldsymbol{Q}_1 \in \mathrm{O}(3)$. If $\boldsymbol{Q}_2 \in \mathrm{O}(3)$ is an element in G_{cr}, we have $w(\boldsymbol{Q}_1) = w(\boldsymbol{Q}_1\boldsymbol{Q}_2)$ for each $\boldsymbol{Q}_1 \in \mathrm{O}(3)$ [18], which leads to equations the texture coefficients of w must satisfy. We distinguish four cases as follows.

Case (1): When both $\boldsymbol{Q}_1$ and $\boldsymbol{Q}_2 \in \mathrm{SO}(3)$, we can write $\boldsymbol{Q}_1 = \boldsymbol{R}_1, \boldsymbol{Q}_2 = \boldsymbol{R}_2 \in \mathrm{SO}(3)$. Then we have $c^{l,R}_{mn} = \sum_{k=-l}^{l} c^{l,R}_{mk} D^l_{nk}(\boldsymbol{R}_2)$.

Proof. Since $w(\boldsymbol{R}_1) = w^R(\boldsymbol{R}_1) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{s=-l}^{l} c^{l,R}_{ms} D^l_{ms}(\boldsymbol{R}_1)$, we have

$$\begin{aligned} w(\boldsymbol{R}_1\boldsymbol{R}_2) = w^R(\boldsymbol{R}_1\boldsymbol{R}_2) &= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} c^{l,R}_{mn} D^l_{mn}(\boldsymbol{R}_1\boldsymbol{R}_2) \\ &= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{n=-l}^{l} c^{l,R}_{mn} \left(\sum_{s=-l}^{l} D^l_{ms}(\boldsymbol{R}_1) D^l_{sn}(\boldsymbol{R}_2) \right) \\ &= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sum_{s=-l}^{l} \left(\sum_{n=-l}^{l} c^{l,R}_{mn} D^l_{sn}(\boldsymbol{R}_2) \right) D^l_{ms}(\boldsymbol{R}_1). \end{aligned} \tag{5.1}$$

Now $w(\boldsymbol{R}_1) = w(\boldsymbol{R}_1\boldsymbol{R}_2)$ implies $c^{l,R}_{ms} = \sum_{n=-l}^{l} c^{l,R}_{mn} D^l_{sn}(\boldsymbol{R}_2)$. By renaming indices, we obtain $c^{l,R}_{mn} = \sum_{k=-l}^{l} c^{l,R}_{mk} D^l_{nk}(\boldsymbol{R}_2)$. □

Case (2): If $\boldsymbol{Q}_1 = \boldsymbol{R}_1 \in \mathrm{SO}(3)$, $\boldsymbol{Q}_2 = \boldsymbol{I}\boldsymbol{R}_2 \in \boldsymbol{I}\mathrm{SO}(3)$, then $c^{l,R}_{mn} = \sum_{k=-l}^{l} c^{l,L}_{mk} D^l_{nk}(\boldsymbol{R}_2)$.

Proof. Since $w(\boldsymbol{R}_1) = w^R(\boldsymbol{R}_1) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\sum_{s=-l}^{l} c_{ms}^{l,R} D_{ms}^{l}(\boldsymbol{R}_1)$, we have

$$\begin{aligned} w(\boldsymbol{R}_1\boldsymbol{Q}_2) = w(\boldsymbol{R}_1\boldsymbol{I}\boldsymbol{R}_2) = w^L(\boldsymbol{R}_1\boldsymbol{R}_2) &= \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\sum_{n=-l}^{l} c_{mn}^{l,L} D_{mn}^{l}(\boldsymbol{R}_1\boldsymbol{R}_2) \\ &= \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\sum_{n=-l}^{l} c_{mn}^{l,L}\left(\sum_{s=-l}^{l} D_{ms}^{l}(\boldsymbol{R}_1) D_{sn}^{l}(\boldsymbol{R}_2)\right) \\ &= \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\sum_{s=-l}^{l}\left(\sum_{n=-l}^{l} c_{mn}^{l,L} D_{sn}^{l}(\boldsymbol{R}_2)\right) D_{ms}^{l}(\boldsymbol{R}_1). \end{aligned} \tag{5.2}$$

Now $w(\boldsymbol{R}_1) = w(\boldsymbol{R}_1\boldsymbol{Q}_2)$ implies $c_{ms}^{l,R} = \sum_{n=-l}^{l} c_{mn}^{l,L} D_{sn}^{l}(\boldsymbol{R}_2)$. By renaming indices, we obtain $c_{mn}^{l,R} = \sum_{k=-l}^{l} c_{mk}^{l,L} D_{nk}^{l}(\boldsymbol{R}_2)$. □

Case (3): If $\boldsymbol{Q}_2 = \boldsymbol{R}_2 \in \mathrm{SO}(3)$, $\boldsymbol{Q}_1 = \boldsymbol{I}\boldsymbol{R}_1 \in \boldsymbol{I}\mathrm{SO}(3)$, then $c_{mn}^{l,L} = \sum_{k=-l}^{l} c_{mk}^{l,L} D_{nk}^{l}(\boldsymbol{R}_2)$.

Proof. We have $w(\boldsymbol{Q}_1) = w(\boldsymbol{I}\boldsymbol{R}_1) = w^L(\boldsymbol{R}_1)$ and $w(\boldsymbol{Q}_1\boldsymbol{Q}_2) = w(\boldsymbol{I}\boldsymbol{R}_1\boldsymbol{R}_2) = w^L(\boldsymbol{R}_1\boldsymbol{R}_2)$. Similar to Case (1), $w^L(\boldsymbol{R}_1) = w^L(\boldsymbol{R}_1\boldsymbol{R}_2)$ implies $c_{mn}^{l,L} = \sum_{k=-l}^{l} c_{mk}^{l,L} D_{nk}^{l}(\boldsymbol{R}_2)$.

Case (4): If $\boldsymbol{Q}_1 = \boldsymbol{I}\boldsymbol{R}_1$, and $\boldsymbol{Q}_2 = \boldsymbol{I}\boldsymbol{R}_2 \in \boldsymbol{I}\mathrm{SO}(3)$, then $c_{mn}^{l,L} = \sum_{k=-l}^{l} c_{mk}^{l,R} D_{nk}^{l}(\boldsymbol{R}_2)$.

Proof. We have $w(\boldsymbol{Q}_1) = w(\boldsymbol{I}\boldsymbol{R}_1) = w^L(\boldsymbol{R}_1)$ and $w(\boldsymbol{Q}_1\boldsymbol{Q}_2) = w(\boldsymbol{I}\boldsymbol{R}_1\boldsymbol{I}\boldsymbol{R}_2) = w^R(\boldsymbol{R}_1\boldsymbol{R}_2)$. Similar to Case (2), $w^L(\boldsymbol{R}_1) = w^R(\boldsymbol{R}_1\boldsymbol{R}_2)$ implies $c_{mn}^{l,L} = \sum_{k=-l}^{l} c_{mk}^{l,R} D_{nk}^{l}(\boldsymbol{R}_2)$.

Notice that $\boldsymbol{Q}_1$ is the orientation of the crystal which can be chosen as $\boldsymbol{Q}_1 \in \mathrm{SO}(3)$ or $\boldsymbol{Q}_1 \in \boldsymbol{I}\mathrm{SO}(3)$. Therefore we can combine Case (1) and Case (3), Case (2) and Case (4) into two cases as follows.

Case (i): For $\boldsymbol{Q}_2 = \boldsymbol{R}_2 \in \mathrm{SO}(3)$, we have

$$c_{mn}^{l,R/L} = \sum_{k=-l}^{l} c_{mk}^{l,R/L} D_{nk}^{l}(\boldsymbol{R}_2); \tag{5.3}$$

Case (ii): For $\boldsymbol{Q}_2 = \boldsymbol{I}\boldsymbol{R}_2 \in \boldsymbol{I}\mathrm{SO}(3)$, we have

$$c_{mn}^{l,R/L} = \sum_{k=-l}^{l} c_{mk}^{l,L/R} D_{nk}^{l}(\boldsymbol{R}_2). \tag{5.4}$$

5.1.2 Texture symmetry

When a polycrystal undergoes a rotation $\boldsymbol{Q}_2 = \boldsymbol{R}_2 \in \mathrm{SO}(3)$, its texture is described by a new ODF $\tilde{w}$, which is related to the ODF w of the polycrystal before rotation by equation $\tilde{w}(\boldsymbol{Q}_1) = w(\boldsymbol{Q}_2^{-1}\boldsymbol{Q}_1)$ for each $\boldsymbol{Q}_1 \in \mathrm{O}(3)$. If $\boldsymbol{Q}_2 = \boldsymbol{R}_2 \in \mathrm{SO}(3)$ is an element in G_{tex} (i.e., the symmetry group of the sample), this yields equations that the texture coefficients must satisfy, namely $c_{mn}^{l,R/L} = \sum_{k=-l}^{l} c_{kn}^{l,R/L} D_{km}^{l}(\boldsymbol{R}_2^{-1})$ [18].

5.2 Restrictions on texture coefficients imposed by crystal symmetries

5.2.1 Crystal Symmetries

For crystal symmetries in O(3), we will discuss restrictions imposed by 32 crystallographic point groups in 3 types by the order listed in Chapter 2.

5.2.1.1 Type I crystal symmetry

In this case, $\boldsymbol{Q}_2 = \boldsymbol{R}_2 \in \mathrm{SO}(3)$, so we have $c_{mn}^{l,R/L} = \sum_{k=-l}^{l} c_{mk}^{l,R/L} D_{nk}^{l}(\boldsymbol{R}_2)$. Let (ψ, θ, ϕ) be the Euler angles pertaining to $\boldsymbol{R}_2^{-1}$. In Roe's notation, we have [20, 32],

$$W_{lmn}^{R/L} = \sqrt{\frac{2}{2l+1}} \sum_{k=-l}^{l} W_{lmk}^{R/L} Z_{lkn}(cos\theta) e^{ik\psi} e^{in\phi}, \tag{5.5}$$

where $W_{lmn}^{R/L} = (-1)^{m-n}\sqrt{\frac{2}{2l+1}} c_{mn}^{l,R/L}$ and $Z_{lmn}(cos\theta) = (-1)^{m-n}\sqrt{\frac{2l+1}{2}} d_{mn}^{l}(\theta)$.

1. C_1

No symmetry for this group. So we won't get any restriction.

2. C_2

Suppose the reference crystal lattice of the crystallites and the spatial coordinate system for the definition of Euler angles are chosen so that the elements of C_2 are $\boldsymbol{E}$ and $\boldsymbol{R}(e_3, \pi)$, where $\boldsymbol{E}$ is the identity. The Euler angles of $\boldsymbol{R}(e_3, \pi)$ are $(0, 0, \pi)$. Then we have $c_{mn}^{l,R/L} =$

$\sum_p c_{mp}^{l,R/L} D_{np}^l(0,0,\pi) = \sum_p c_{mp}^{l,R/L} d_{np}^l(0)e^{-ip\pi} = c_{mn}^{l,R/L}\cos(n\pi)$ [18]. Thus $c_{mn}^{l,R/L} = 0$ if n is odd or $W_{lmn}^{R/L} = 0$ if n is odd.

3. C_3

Suppose the reference crystal lattice of the crystallites and the spatial coordinate system for the definition of Euler angles are chosen so that the elements are $\boldsymbol{E}$, $\boldsymbol{R}(e_3, \frac{2\pi}{3})$ and $\boldsymbol{R}(e_3, \frac{4\pi}{3})$, with $\boldsymbol{R}(e_3, \frac{2\pi}{3})$ being the generator with Euler angles given by $(0, 0, \frac{2\pi}{3})$. Then we have

$$c_{mn}^{l,R/L} = \sum_p c_{mp}^{l,R/L} D_{np}^l(0,0,\frac{2\pi}{3}) = \sum_p c_{mp}^{l,R/L} d_{np}^l(0)e^{\frac{-2ip\pi}{3}} = c_{mn}^{l,R/L}\cos(\frac{2n\pi}{3}). \tag{5.6}$$

Hence $c_{mn}^{l,R/L} = 0$ for $n \neq 3k$, $k \in \mathbb{Z}$, or $W_{lmn}^{R/L} = 0$ for $n \neq 3k$, $k \in \mathbb{Z}$.

4. C_4

Suppose the reference crystal lattice of the crystallites and the spatial coordinate system for the definition of Euler angles are chosen so that the elements are generated by $\boldsymbol{R}(e_3, \frac{\pi}{2})$. Similarly, we have $c_{mn}^{l,R/L} = 0$ for $n \neq 4k$, $k \in \mathbb{Z}$, or $W_{lmn}^{R/L} = 0$ for $n \neq 4k$, $k \in \mathbb{Z}$.

5. C_6

Suppose the reference crystal lattice of the crystallites and the spatial coordinate system for the definition of Euler angles are chosen so that the elements are generated by $\boldsymbol{R}(e_3, \frac{\pi}{3})$. We then have $c_{mn}^{l,R/L} = 0$ for $n \neq 6k$, $k \in \mathbb{Z}$, or $W_{lmn}^{R/L} = 0$ for $n \neq 6k$, $k \in \mathbb{Z}$.

6. D_2

Suppose the reference crystal lattice of the crystallites and the spatial coordinate system for the definition of Euler angles are chosen so that the elements of D_2 are $\boldsymbol{E}$, $\boldsymbol{R}(e_1, \pi)$, $\boldsymbol{R}(e_2, \pi)$ and $\boldsymbol{R}(e_3, \pi)$. Orthorhombic crystal symmetry dictates that $\tilde{c}_{mn}^l = c_{mn}^l$ for $\boldsymbol{R}$ given by the Euler angles $(0, \pi, 0)$, $(0, 0, \pi)$, and $(0, \pi, \pi)$, respectively. Clearly only two of them are independent.

For $\boldsymbol{R}(e_2,\pi)$ given by Euler angle $(0,\pi,0)$, we have [18]

$$c_{mn}^{l,R/L} = \sum_p c_{mp}^{l,R/L} D_{np}^l(0,\pi,0) = \sum_p c_{mp}^{l,R/L} d_{np}^l(\pi) = \sum_p c_{mp}^{l,R/L}(-1)^{l+n} d_{n\bar{p}}^l(0) = (-1)^{l+n} c_{m\bar{n}}^{l,R/L}. \tag{5.7}$$

Note that $d_{mn}^l(0) = \delta_{mn}$. Thus we obtain $c_{mn}^{l,R/L} = (-1)^{l+n} c_{m\bar{n}}^{l,R/L}$.

For $\boldsymbol{R}(e_3,\pi)$ given by $(0,0,\pi)$, we have [18]

$$c_{mn}^{l,R/L} = \sum_p c_{mp}^{l,R/L} D_{np}^l(0,0,\pi) = \sum_p c_{mp}^{l,R/L} d_{np}^l(0) e^{-ip\pi} = c_{mn}^{l,R/L}\cos(n\pi). \tag{5.8}$$

Therefore $c_{mn}^{l,R/L} = 0$ if n is odd, or $W_{lmn}^{R/L} = 0$ if n is odd.

Combining the preceding two requirements, we have

$$c_{mn}^{l,R/L} = \begin{cases} (-1)^l c_{m\bar{n}}^{l,R/L}, & \text{for even } n; \\ 0, & \text{for odd } n. \end{cases} \tag{5.9}$$

7. D_3

Suppose the reference crystal lattice of the crystallites and the spatial coordinate system for the definition of Euler angles are chosen so that the elements are generated by $\boldsymbol{R}(e_3,\frac{2\pi}{3})$ and $\boldsymbol{R}(e_2,\pi)$. As discussed earlier, $\boldsymbol{R}(e_3,\frac{2\pi}{3})$ implies $c_{mn}^{l,R/L} = 0$ for $n \neq 3k$, $k \in \mathbb{Z}$; and $\boldsymbol{R}(e_2,\pi)$ implies $c_{mn}^{l,R/L} = (-1)^{l+n} c_{m\bar{n}}^{l,R/L}$.

Combining these two, we have

$$c_{mn}^{l,R/L} = \begin{cases} (-1)^{l+n} c_{m\bar{n}}^{l,R/L}, & \text{for } n = 3k, k \in \mathbb{Z}; \\ 0, & \text{else.} \end{cases} \tag{5.10}$$

8. D_4

Suppose the reference crystal lattice of the crystallites and the spatial coordinate system for the definition of Euler angles are chosen so that the elements are generated by $\boldsymbol{R}(e_3,\frac{\pi}{2})$

and $\boldsymbol{R}(e_2, \pi)$. Similar to the discussions on D_2 and D_3, we have

$$c_{mn}^{l,R/L} = \begin{cases} (-1)^l c_{m\bar{n}}^{l,R/L}, & \text{for } n = 4k, k \in \mathbb{Z}; \\ 0, & \text{else.} \end{cases} \tag{5.11}$$

9. D_6

Suppose the reference crystal lattice of the crystallites and the spatial coordinate system for the definition of Euler angles are chosen so that the elements are generated by $\boldsymbol{R}(e_3, \frac{\pi}{3})$ and $\boldsymbol{R}(e_2, \pi)$. Likewise, we have

$$c_{mn}^{l,R/L} = \begin{cases} (-1)^l c_{m\bar{n}}^{l,R/L}, & \text{for } n = 6k, k \in \mathbb{Z}; \\ 0, & \text{else.} \end{cases} \tag{5.12}$$

10. T

Suppose the reference crystal lattice of the crystallites and the spatial coordinate system for the definition of Euler angles are chosen so that the elements are generated by $\boldsymbol{R}(e_3, \pi)$, $\boldsymbol{R}(e_2, \pi)$, and $\boldsymbol{R}(n, \frac{2\pi}{3})$, where $n = \frac{1}{\sqrt{3}}(e_1 + e_2 + e_3)$. We can write $\boldsymbol{R}(n, \frac{2\pi}{3}) = \boldsymbol{R}(e_2, \frac{\pi}{2})R(e_3, \frac{\pi}{2})$. Invariance under $\boldsymbol{R}(e_3, \pi)$ implies $c_{mn}^{l,R/L} = 0$ if n is odd, and invariance under $\boldsymbol{R}(e_2, \pi)$ implies $c_{mn}^{l,R/L} = (-1)^{l+n} c_{m\bar{n}}^{l,R/L}$. Combining the preceding two requirements as in D_2, we have

$$c_{mn}^{l,R/L} = \begin{cases} (-1)^l c_{m\bar{n}}^{l,R/L}, & \text{for even } n; \\ 0, & \text{for odd } n. \end{cases} \tag{5.13}$$

Next invariance under $\boldsymbol{R}(e_2, \frac{\pi}{2})\boldsymbol{R}(e_3, \frac{\pi}{2})$ implies [18]

$$c_{mn}^{l,R/L} = \sum_p c_{mp}^{l,R/L} D_{np}^l(0, \frac{\pi}{2}, \frac{\pi}{2}) = \sum_p c_{mp}^{l,R/L} d_{np}^l(\frac{\pi}{2}) e^{\frac{-ip\pi}{2}} = \sum_p c_{mp}^{l,R/L} d_{np}^l(\frac{\pi}{2}) \cos(\frac{p\pi}{2}), \tag{5.14}$$

where p is even.

With the fact that [18]

$$c_{m\bar{p}}^{l,R/L} d_{n\bar{p}}^l(\frac{\pi}{2}) = (-1)^l c_{mn}^{l,R/L} (-1)^{l+n} d_{np}^l(\frac{\pi}{2}) = c_{mn}^{l,R/L} d_{np}^l(\frac{\pi}{2}) \tag{5.15}$$

for even p, we may recast (5.14) in the following form:

$$\begin{pmatrix} d^l_{00}(\frac{\pi}{2})-1, & -2d^l_{02}(\frac{\pi}{2}), & \ldots, & (-1)^{\frac{p}{2}}2d^l_{0p}(\frac{\pi}{2}), & \ldots, & (-1)^{\frac{N}{2}}2d^l_{0N}(\frac{\pi}{2}) \\ d^l_{20}(\frac{\pi}{2}), & -2d^l_{22}(\frac{\pi}{2})-1, & \ldots, & (-1)^{\frac{p}{2}}2d^l_{2p}(\frac{\pi}{2}), & \ldots, & (-1)^{\frac{N}{2}}2d^l_{2N}(\frac{\pi}{2}) \\ \ldots, & \ldots, & \ldots, & \ldots, & \ldots, & \ldots \\ \ldots, & \ldots, & \ldots, & \ldots, & \ldots, & \ldots \\ d^l_{N0}(\frac{\pi}{2}), & -2d^l_{N2}(\frac{\pi}{2}), & \ldots, & (-1)^{\frac{p}{2}}2d^l_{Np}(\frac{\pi}{2}), & \ldots, & (-1)^{\frac{N}{2}}2d^l_{NN}(\frac{\pi}{2})-1 \end{pmatrix} \begin{pmatrix} c^{l,R/L}_{m0} \\ c^{l,R/L}_{m2} \\ c^{l,R/L}_{m4} \\ \ldots \\ c^{l,R/L}_{mN} \end{pmatrix} = \mathbf{0} \quad (5.16)$$

Here N is the largest positive even integer that satisfies $N \leq l$. With equations (5.13) and (5.16), we list the exact relations on $W^{R/L}_{lmn}$ for $l \leq 12$ in Table 5.1. Here we use $W^{R/L}_{lmn}$ as the texture coefficients instead of $c^{l,R/L}_{mn}$ to match the notations in [18]. Note that $W^{R/L}_{lmn} = (-1)^{m-n}\sqrt{\frac{2}{2l+1}}c^{l,R/L}_{mn}$. These relations are obtained through a simple Maple program, which delivers also the exact relations for the higher l's. With increasing l, however, the exact relations soon become too complicated and unwisely for practical use.

Table 5.1: Relations on the texture coefficients W_{lmn} for aggregates of tetrahedral (T) crystallites for $1 \leq l \leq 12$.

l	Lin. indep. coeff.	Lin dep. coeff.
2		$W_{2m0} = W_{2m2} = 0$
3	W_{3m2}	
4	W_{4m0}	$W_{4m4} = \frac{\sqrt{70}}{14} W_{4m0}$
6	W_{6m0}	$W_{6m4} = -\frac{\sqrt{14}}{2} W_{6m0}$
	W_{6m2}	$W_{6m6} = -\frac{\sqrt{55}}{11} W_{6m2}$
7	W_{7m2}	$W_{7m6} = \frac{\sqrt{143}}{13} W_{7m2}$
8	W_{8m0}	$W_{8m4} = \frac{\sqrt{154}}{33} W_{8m0}$
		$W_{8m8} = \frac{\sqrt{1430}}{66} W_{8m0}$
9	W_{9m2}	$W_{9m6} = -\frac{\sqrt{39}}{3} W_{9m2}$
	W_{9m4}	$W_{9m8} = -\frac{\sqrt{119}}{17} W_{9m4}$
10	W_{10m0}	$W_{10m4} = -\frac{\sqrt{4290}}{65} W_{10m0}$
		$W_{10m8} = -\frac{\sqrt{24310}}{130} W_{10m0}$
	W_{10m2}	$W_{10m6} = \frac{\sqrt{26}}{26} W_{10m2}$
		$W_{10m10} = -\frac{\sqrt{125970}}{494} W_{10m2}$
11	W_{11m2}	$W_{11m6} = \frac{\sqrt{22610}}{170} W_{11m2}$
		$W_{11m10} = \frac{9\sqrt{170}}{170} W_{11m2}$
12	W_{12m0}	$W_{12m8} = \frac{\sqrt{277134}}{646} W_{12m0} - \frac{4\sqrt{13566}}{323} W_{12m4}$
	W_{12m4}	$W_{12m12} = \frac{4\sqrt{676039}}{7429} W_{12m0} + \frac{9\sqrt{81719}}{7429} W_{12m4}$
	W_{12m2}	$W_{12m6} = -\frac{5\sqrt{714}}{34} W_{12m2}$
		$W_{12m10} = \frac{\sqrt{7106}}{34} W_{12m2}$

Note: $W^{R/L}_{lmn} = (-1)^l W^{R/L}_{lm\bar{n}}$. For those $1 \leq l \leq 12$ not given in the table, all $W_{lmn} = 0$. Also, $W_{lmn} = 0$ for odd l. For brevity, we write W for $W^{R/L}$ in the table.

11. O

Suppose the reference crystal lattice of the crystallites and the spatial coordinate system for the definition of Euler angles are chosen so that the elements are generated by $\boldsymbol{R}(e_1, \frac{\pi}{2})$, $\boldsymbol{R}(e_2, \frac{\pi}{2})$, and $\boldsymbol{R}(e_3, \frac{\pi}{2})$.

As in D_4, invariance under $\boldsymbol{R}(e_2, \pi)$ and $\boldsymbol{R}(e_3, \frac{\pi}{2})$ imply

$$c_{mn}^{l,R/L} = \begin{cases} (-1)^l c_{m\bar{n}}^{l,R/L}, & \text{for } n = 4k, k \in \mathbb{Z}; \\ 0, & \text{else.} \end{cases} \tag{5.17}$$

The restrictions imposed by $\boldsymbol{R}(e_2, \frac{\pi}{2})$ implies [18]

$$c_{mn}^{l,R/L} = \sum_p c_{mp}^{l,R/L} D_{np}^l(0, \frac{\pi}{2}, 0) = \sum_p c_{mp}^{l,R/L} d_{np}^l(\frac{\pi}{2}) \tag{5.18}$$

where p is $p = 4k$, $k \in \mathbb{Z}$.

Again with the fact that

$$c_{m\bar{p}}^{l,R/L} d_{n\bar{p}}^l(\frac{\pi}{2}) = (-1)^l c_{mn}^{l,R/L} (-1)^{l+n} d_{np}^l(\frac{\pi}{2}) = c_{mn}^{l,R/L} d_{np}^l(\frac{\pi}{2}) \tag{5.19}$$

for even p, we may recast (5.18) in the following form:

$$\begin{pmatrix} d_{00}^l(\frac{\pi}{2}) - 1, & 2d_{04}^l(\frac{\pi}{2}), & \ldots, & 2d_{0N}^l(\frac{\pi}{2}) \\ d_{40}^l(\frac{\pi}{2}), & 2d_{44}^l(\frac{\pi}{2}) - 1, & \ldots, & 2d_{4N}^l(\frac{\pi}{2}) \\ \ldots, & \ldots, & \ldots, & \ldots \\ \ldots, & \ldots, & \ldots, & \ldots \\ d_{N0}^l(\frac{\pi}{2}), & 2d_{N4}^l(\frac{\pi}{2}), & \ldots, & 2d_{NN}^l(\frac{\pi}{2}) - 1 \end{pmatrix} \begin{pmatrix} c_{m0}^{l,R/L} \\ c_{m4}^{l,R/L} \\ c_{m8}^{l,R/L} \\ \ldots \\ c_{mN}^{l,R/L} \end{pmatrix} = \mathbf{0}. \tag{5.20}$$

Here N is the largest positive integer that satisfies $N \leq l$ and $N = 4k$ for some integer k. With equations (5.17) and (5.20), we can calculate the exact relations for $l \leq 15$ through a simple Maple program [18]. The results are displayed in Table 5.2.

Table 5.2: Relations on the texture coefficients W_{lmn} for aggregates of cubic (O) crystallites for $1 \leq l \leq 15$.

l	Lin. indep. coeff.	Lin dep. coeff.
4	W_{4m0}	$W_{4m4} = \frac{\sqrt{70}}{14} W_{4m0}$
6	W_{6m0}	$W_{6m4} = -\frac{\sqrt{14}}{2} W_{6m0}$
8	W_{8m0}	$W_{8m4} = \frac{\sqrt{154}}{33} W_{8m0}$
		$W_{8m8} = \frac{\sqrt{1430}}{66} W_{8m0}$
9	W_{9m4}	$W_{9m8} = -\frac{\sqrt{119}}{17} W_{9m4}$
10	W_{10m0}	$W_{10m4} = -\frac{\sqrt{4290}}{65} W_{10m0}$
		$W_{10m8} = -\frac{\sqrt{24310}}{130} W_{10m0}$
12	W_{12m0}	$W_{12m8} = \frac{\sqrt{277134}}{646} W_{12m0} - \frac{4\sqrt{13566}}{323} W_{12m4}$
	W_{12m4}	$W_{12m12} = \frac{4\sqrt{676039}}{7429} W_{12m0} + \frac{9\sqrt{81719}}{7429} W_{12m4}$
13	W_{13m4}	$W_{13m8} = 2\frac{\sqrt{190}}{95} W_{13m4}$
		$W_{13m12} = -\frac{\sqrt{4807}}{95} W_{13m4}$
14	W_{14m0}	$W_{14m4} = -3\frac{\sqrt{85085}}{1190} W_{14m0}$
		$W_{14m8} = -\frac{\sqrt{881790}}{1190} W_{14m0}$
		$W_{14m12} = -\frac{\sqrt{52003}}{238} W_{14m0}$
15	W_{15m4}	$W_{15m8} = -2\frac{\sqrt{966}}{23} W_{15m4}$
		$W_{15m12} = \frac{\sqrt{1495}}{23} W_{15m4}$

Note: $W^{R/L}_{lmn} = (-1)^l W^{R/L}_{lm\bar{n}}$. For those $1 \leq l \leq 15$ not given in the table, all $W_{lmn} = 0$. Also, $W_{lmn} = 0$ for odd l. For brevity, we write W for $W^{R/L}$ in the table.

5.2.1.2 Type II crystal symmetry

Each $G_{\rm cr}$ of Type II contains the inversion $\boldsymbol{I}$ as an element and can be written as $G_{cr} = G_p \cup \boldsymbol{I}G_p$, where G_p is of Type I. For an ODF $w : \mathrm{O}(3) \to \mathbb{R}^1$, we have

$$w^R(\boldsymbol{R}) = w(\boldsymbol{R}) = w(\boldsymbol{RI}) = w(\boldsymbol{IR}) = w^L(\boldsymbol{R}) \qquad \text{for } \boldsymbol{R} \in \mathrm{SO}(3).$$

It follows that $c^{l,R}_{mn} = c^{l,L}_{mn}$ or in Roe's notation, $W^R_{lmn} = W^L_{lmn}$. Hence the restrictions imposed by $G_{\rm cr} = G_p \cup \boldsymbol{I}G_p$ of Type II on the texture coefficients $c^{l,R/L}_{mn}$ or $W^{R/L}_{lmn}$ are exactly the same as those imposed by the proper subgroup G_p on the texture coefficients c^l_{mn} or W_{lmn} reported in Section 5.2.1.1.

5.2.1.3 Type III crystal symmetry

As in Chapter 2, the 10 improper groups G_i in Type III, which do not contain the inversion as an element, are:

$$C_s, C_{2v}, S_4, C_{4v}, D_{2d}, C_{3v}, C_{3h}, D_{3h}, C_{6v}, T_d. \tag{5.21}$$

For each of these groups, the subset with the identity and all rotational elements form a subgroup G_p. And the proper rotational subgroups G_p, in the order of G_i listed above, are:

$$C_1, C_2, C_2, C_4, D_2, C_3, C_3, D_3, C_6, T \tag{5.22}$$

Since $G_i = G_p \cup \bar{\boldsymbol{R}}_2 G_p = G_p \cup \boldsymbol{I}\boldsymbol{R}_2 G$ for some specific rotation $\boldsymbol{R}_2 \notin G_p$, the restrictions imposed by G_i on texture coefficients are exactly those imposed by G_p and the extra generator $\boldsymbol{Q}_2 = \bar{\boldsymbol{R}}_2 = \boldsymbol{I}\boldsymbol{R}_2 \in \boldsymbol{I}\mathrm{SO}(3)$. The corresponding rotational subgroup G_p and rotation $\boldsymbol{R}_2$ pertaining to each improper group G_i in Type III are listed in Table 5.3.

Notice that both C_{2v} and S_4 have C_2 as the rotational subgroup, but their W^R_{lmn} and W^L_{lmn} (or, $c^{l,R}_{mn}$ and $c^{l,L}_{mn}$) are related differently. Similarly, C_{3v} and C_{3h} both have C_3 as the rotational subgroup.

Table 5.3: Corresponding rotational subgroup G_p and $\boldsymbol{R}_2$ of each Type III improper group G_i.

Improper group G_i	Rotational subgroup G_p	$\boldsymbol{R}_2$
C_s	C_1	$\boldsymbol{R}(e_3, \pi)$
C_{2v}	C_2	$\boldsymbol{R}(e_2, \pi)$
S_4	C_2	$\boldsymbol{R}(e_3, \frac{\pi}{2})$
C_{4v}	C_4	$\boldsymbol{R}(e_2, \pi)$
D_{2d}	D_2	$\boldsymbol{R}(e_3, \frac{\pi}{2})$
C_{3v}	C_3	$\boldsymbol{R}(e_2, \pi)$
C_{3h}	C_3	$\boldsymbol{R}(e_3, \frac{\pi}{3})$
D_{3h}	D_3	$\boldsymbol{R}(e_3, \frac{\pi}{3})$
C_{6v}	C_6	$\boldsymbol{R}(e_2, \frac{\pi}{2})$
T_d	T	$\boldsymbol{R}(e_3, \frac{\pi}{2})$

Note: $G_i = G_p \cup \bar{\boldsymbol{R}}_2 G_p$ (e.g. $C_s = C_1 \cup \bar{\boldsymbol{R}}_2 C_1$, where $\bar{\boldsymbol{R}}_2 = \boldsymbol{IR}(e_3, \pi)$).

Next we will discuss these 10 improper groups separately as crystal symmetries.

1. C_s, S_1 or C_{1h}

Suppose the reference crystal lattice of the crystallites and the spatial coordinate system for the definition of Euler angles are chosen so that the elements are $\boldsymbol{E}$ and $\boldsymbol{IR}(e_3, \pi)$.

Invariance under $\boldsymbol{IR}(e_3, \pi)$ with $\boldsymbol{R}(e_3, \pi)$ given by $(0, 0, \pi)$ implies

$$c_{mn}^{l,R/L} = \sum_p c_{mp}^{l,L/R} D_{np}^l(0, 0, \pi) = \sum_p c_{mp}^{l,L/R} d_{np}^l(0) e^{-ip\pi} = c_{mn}^{l,L/R} \cos(n\pi) = (-1)^n c_{mn}^{l,L/R}. \quad (5.23)$$

Thus

$$c_{mn}^{l,R/L} = \begin{cases} c_{mn}^{l,L/R}, & \text{for even } n; \\ -c_{mn}^{l,L/R}, & \text{for odd } n. \end{cases} \quad (5.24)$$

2. S_4

Suppose the reference crystal lattice of the crystallites and the spatial coordinate system for the definition of Euler angles are chosen so that the elements are $\boldsymbol{E}$, $\boldsymbol{R}(e_3, \pi)$, $\boldsymbol{IR}(e_3, \frac{\pi}{2})$ and $\boldsymbol{IR}(e_3, \frac{3\pi}{2})$. Invariance under $\boldsymbol{R}(e_3, \pi)$ implies that texture coefficients are zero unless n is even (as in C_2). Invariance under $\boldsymbol{IR}(e_3, \frac{\pi}{2})$ implies

$$c_{mn}^{l,R/L} = \sum_p c_{mp}^{l,L/R} D_{np}^l(0, 0, \frac{\pi}{2}) = \sum_p c_{mp}^{l,L/R} d_{np}^l(0) e^{-\frac{ip\pi}{2}} = c_{mn}^{l,L/R} \cos(\frac{n\pi}{2}) = (-1)^{\frac{n}{2}} c_{mn}^{l,L/R}. \quad (5.25)$$

Together we have,

$$c_{mn}^{l,R/L} = \begin{cases} c_{mn}^{l,L/R}, & \text{for } n = 4k, k \in \mathbb{Z}; \\ -c_{mn}^{l,L/R}, & \text{for } n = 4k+2, k \in \mathbb{Z}; \\ 0, & \text{else.} \end{cases} \quad (5.26)$$

3. C_{3h}

Suppose the reference crystal lattice of the crystallites and the spatial coordinate system for the definition of Euler angles are chosen so that the elements are generated by $\boldsymbol{IR}(e_3, \frac{\pi}{3})$. Clearly , $\boldsymbol{R}(e_3, \frac{2\pi}{3})$ is also an element which implies, as in C_3, $n = 3k, k \in \mathbb{Z}$ for non-zero texture coefficients. Invariance under $\boldsymbol{IR}(e_3, \frac{\pi}{3})$ implies

$$c_{mn}^{l,R/L} = \sum_p c_{mp}^{l,L/R} D_{np}^l(0, 0, \frac{\pi}{3}) = \sum_p c_{mp}^{l,L/R} d_{np}^l(0) e^{-\frac{ip\pi}{3}} = c_{mn}^{l,L/R} \cos(\frac{n\pi}{3}) = (-1)^{\frac{n}{3}} c_{mn}^{l,L/R}. \quad (5.27)$$

Therefore,

$$c_{mn}^{l,R/L} = \begin{cases} c_{mn}^{l,L/R}, & \text{for } n = 6k, k \in \mathbb{Z}; \\ -c_{mn}^{l,L/R}, & \text{for } n = 6k+3, k \in \mathbb{Z}; \\ 0, & \text{else.} \end{cases} \tag{5.28}$$

4. C_{2v}

Suppose the reference crystal lattice of the crystallites and the spatial coordinate system for the definition of Euler angles are chosen so that we can write

$$C_{2v} = \{e, \boldsymbol{R}(e_3, \pi), \boldsymbol{IR}(e_2, \pi), \boldsymbol{IR}(e_1, \pi)\}. \tag{5.29}$$

Invariance under $\boldsymbol{R}(e_3, \pi)$ implies that n must be even for non-zero $c_{mn}^{l,R/L}$ as in C_2. Invariance under $\boldsymbol{IR}(e_2, \pi)$ with Euler anger $(0, \pi, 0)$ implies $c_{mn}^{l,R/L} = (-1)^{l+n} c_{m\bar{n}}^{l,L/R}$ with similar argument indicated in (5.7).

Together we have

$$c_{mn}^{l,R/L} = \begin{cases} (-1)^l c_{m\bar{n}}^{l,L/R}, & \text{for even } n; \\ 0, & \text{for odd } n. \end{cases} \tag{5.30}$$

5. C_{3v}

Suppose the reference crystal lattice of the crystallites and the spatial coordinate system for the definition of Euler angles are chosen so that the elements are generated by $\boldsymbol{R}(e_3, \frac{2\pi}{3})$ and $\boldsymbol{IR}(e_2, \pi)$. Invariance under $\boldsymbol{R}(e_3, \frac{2\pi}{3})$ implies, as in C_3, $n = 3k, k \in \mathbb{Z}$ for non-zero texture coefficients. Invariance under $\boldsymbol{IR}(e_2, \pi)$ implies $c_{mn}^{l,R/L} = (-1)^{l+n} c_{m\bar{n}}^{l,L/R}$. Thus

$$c_{mn}^{l,R/L} = \begin{cases} (-1)^l c_{m\bar{n}}^{l,L/R}, & \text{for } n = 6k, k \in \mathbb{Z}; \\ (-1)^{l+1} c_{m\bar{n}}^{l,L/R}, & \text{for } n = 6k+3, k \in \mathbb{Z}; \\ 0, & \text{else.} \end{cases} \tag{5.31}$$

6. C_{4v}

Suppose the reference crystal lattice of the crystallites and the spatial coordinate system for the definition of Euler angles are chosen so that the elements are generated by $\boldsymbol{R}(e_3, \frac{\pi}{2})$ and $\boldsymbol{IR}(e_2, \pi)$. We can write $C_{4v} = C_4 \bigcup \bar{C}_2 C_4$. Invariance under $\boldsymbol{R}(e_3, \frac{\pi}{2})$ with Euler anger $(0, 0, \frac{\pi}{2})$ implies $n = 4k, k \in \mathbb{Z}$ for non-zero texture coefficients; invariance under $\boldsymbol{IR}(e_2, \pi)$ implies $c_{mn}^{l,R/L} = (-1)^{l+n} c_{m\bar{n}}^{l,L/R}$. We then have

$$c_{mn}^{l,R/L} = \begin{cases} (-1)^l c_{m\bar{n}}^{l,L/R}, & \text{for } n = 4k, k \in \mathbb{Z}; \\ 0, & \text{else.} \end{cases} \tag{5.32}$$

7. D_{2d}

Suppose the reference crystal lattice of the crystallites and the spatial coordinate system for the definition of Euler angles are chosen so that the elements are generated by $\boldsymbol{R}(e_2, \pi)$, $\boldsymbol{R}(e_3, \pi)$, and $\boldsymbol{IR}(e_3, \frac{\pi}{2})$. Invariance under $\boldsymbol{IR}(e_3, \frac{\pi}{2})$ implies $c_{mn}^{l,R/L} = (-1)^{n/2} c_{mn}^{l,L/R}$. Combining this with the restrictions imposed by D_2, we have:

(1) if $n = 4k$ for some integer k, then $c_{mn}^{l,R} = c_{mn}^{l,L}$ and we have $c_{mn}^{l,R/L} = (-1)^l c_{m\bar{n}}^{l,R/L}$;

(2) if $n = 4k+2$ for some integer k, then $c_{mn}^{l,R} = -c_{mn}^{l,L}$ and we also have $c_{mn}^{l,R/L} = (-1)^l c_{m\bar{n}}^{l,R/L}$.

8. C_{6v}

Suppose the reference crystal lattice of the crystallites and the spatial coordinate system for the definition of Euler angles are chosen so that the elements are generated by $\boldsymbol{R}(e_3, \frac{\pi}{3})$ and $\boldsymbol{IR}(e_2, \pi)$. As in C_6, invariance under $\boldsymbol{R}(e_3, \frac{\pi}{3})$ implies that $n = 6k, k \in \mathbb{Z}$ for non-zero texture coefficients. Invariance under $\boldsymbol{IR}(e_2, \pi)$ implies $c_{mn}^{l,R/L} = (-1)^{l+n} c_{m\bar{n}}^{l,L/R}$.

Combining these requirements, we obtain

$$c_{mn}^{l,R/L} = \begin{cases} (-1)^l c_{m\bar{n}}^{l,L/R}, & \text{for } n = 6k, k \in \mathbb{Z}; \\ 0, & \text{else.} \end{cases} \tag{5.33}$$

9. D_{3h}

Suppose the reference crystal lattice of the crystallites and the spatial coordinate system for the definition of Euler angles are chosen so that the elements are generated by $\boldsymbol{IR}(e_3, \frac{\pi}{3})$ and $\boldsymbol{R}(e_2, \pi)$. Notice that we can write $D_{3h} = D_3 \bigcup \bar{\boldsymbol{R}} D_3$ with $\boldsymbol{R} = \boldsymbol{R}(e_3, \frac{\pi}{3})$.

The restrictions imposed by D_3 is:

$$c_{mn}^{l,R/L} = \begin{cases} (-1)^{l+n} c_{m\bar{n}}^{l,R/L}, & \text{for } n = 3k, k \in \mathbb{Z}; \\ 0 \quad , & \text{else.} \end{cases} \tag{5.34}$$

Invariance under $\boldsymbol{IR}(e_3, \frac{\pi}{3})$ implies

$$c_{mn}^{l,R/L} = \sum_p c_{mp}^{l,L/R} D_{np}^l(0, 0, \frac{\pi}{3}) = \sum_p c_{mp}^{l,L/R} d_{np}^l(0) e^{-\frac{ip\pi}{3}} = c_{mn}^{l,L/R} \cos(\frac{n\pi}{3}) = (-1)^{\frac{n}{3}} c_{mn}^{l,L/R}. \tag{5.35}$$

In conclusion, we have:

(1) if $n = 6k$ for some integer k, then $c_{mn}^{l,R} = c_{mn}^{l,L}$ and we have $c_{mn}^{l,R/L} = (-1)^l c_{m\bar{n}}^{l,R/L}$;

(2) if $n = 6k + 3$ for some integer k, then $c_{mn}^{l,R} = -c_{mn}^{l,L}$ and $c_{mn}^{l,R/L} = (-1)^{l+1} c_{m\bar{n}}^{l,R/L}$.

10. T_d

Suppose the reference crystal lattice of the crystallites and the spatial coordinate system for the definition of Euler angles are chosen so that the elements are generated by $\boldsymbol{R}(e_3, \pi)$, $\boldsymbol{R}(e_2, \pi)$, $\boldsymbol{R}(e_2, \frac{\pi}{2})\boldsymbol{R}(e_3, \frac{\pi}{2})$ and $\boldsymbol{IR}(e_3, \frac{\pi}{2})$. Here $\boldsymbol{R}(e_2, \frac{\pi}{2})\boldsymbol{R}(e_3, \frac{\pi}{2}) = \boldsymbol{R}(n, \frac{2\pi}{3})$, where $n = \frac{1}{\sqrt{3}}(e_1 + e_2 + e_3)$.

Invariance under $\boldsymbol{IR}(e_3, \frac{\pi}{2})$ implies

$$c_{mn}^{l,R/L} = \sum_p c_{mp}^{l,L/R} D_{np}^l(0, 0, \frac{\pi}{2}) = \sum_p c_{mp}^{l,L/R} d_{np}^l(0) e^{-\frac{ip\pi}{2}} = c_{mn}^{l,L/R} \cos(\frac{n\pi}{2}). \tag{5.36}$$

Invariance under $\boldsymbol{R}(e_3, \pi)$ implies that n is even for non-zero c_{mn}^l. Thus $c_{mn}^{l,R/L} = (-1)^{\frac{n}{2}} c_{mn}^{l,L/R}$ for even n.

Combining the restrictions above with those imposed by T, we have:

(1) if $n = 4k$ for some integer k, then $c^{l,R}_{mn} = c^{l,L}_{mn}$;

(2) if $n = 4k + 2$ for some integer k, then $c^{l,R}_{mn} = -c^{l,L}_{mn}$.

In both cases, we have $c^{l,R/L}_{mn} = (-1)^l c^{l,R/L}_{m\bar{n}}$ and the results listed in Table 5.1.

Remark: Material symmetries defined by the 32 crystallographic point groups can be distinguished by their restrictions on the texture coefficients of w^R and w^L. The lowest order p such that all crystallographic point groups can be distinguished by c^l_{mn} or W_{lmn} with $l \le p$ is 4, i.e. with l no more than 4, the non-zero c^l_{mn} or W_{lmn} coefficients under each group are different or differently related. For example, to distinguish the point groups T and O, we see that c^3_{m2} or $W_{3m2} \neq 0$ for T and c^3_{m2} or $W_{3m2} = 0$ for O.

5.2.2 Texture symmetry

Here we just consider the case where G_{tex} is of Type I, i.e., G_{tex} is a subgroup of SO(3). As in Sec 5.1.2, we have $w^R(\boldsymbol{R}_1) = w^R(\boldsymbol{R}_2^{-1}\boldsymbol{R}_1)$ and $w^L(\boldsymbol{R}_1) = w^L(\boldsymbol{R}_2^{-1}\boldsymbol{R}_1)$, for each $\boldsymbol{R}_2 \in G_{\text{tex}}$ and $\boldsymbol{R}_1 \in \text{SO}(3)$.

We then have [18],

$$c^{l,R/L}_{mn} = \sum_{p=-l}^{l} c^{l,R/L}_{pn} D^l_{pm}(\boldsymbol{R}_2^{-1}); \tag{5.37}$$

or in Roe's notation,

$$W^{R/L}_{lmn} = \sqrt{\frac{2}{2l+1}} \sum_{k=-l}^{l} W^{R/L}_{lkn} Z_{lkm}(\cos\theta) e^{-ik\psi} e^{-in\phi}. \tag{5.38}$$

Here $c^{l,R/L}_{mn}$ and $W^{R/L}_{lmn}$ are texture coefficients, and $W^{R/L}_{lmn} = (-1)^{m-n}\sqrt{\frac{2}{2l+1}} c^{l,R/L}_{mn}$.

The restrictions imposed by sample symmetries can be found simply by exchanging m and n in the restrictions imposed by crystal symmetries.

Chapter 6 An application of the extended representation theorem

The representation formulas derived in Chapter 4 are meant for material tensors and pseudotensors of weakly-textured polycrystals. But they are valid also for the special case where the crystallites all have the same orientation. This special case covers also single crystals which are weakly anisotropic. Given a single crystal with a particular G_{cr} and a certain rth-order material tensor or pseudotensor $\boldsymbol{H}$ pertaining to the crystal, information such as restrictions imposed by crystal symmetry on the components of $\boldsymbol{H}$ and the number of undetermined material parameters (UMPs) carried by it, which do not depend on whether the anisotropy of the crystal is strong or weak, can be determined by the representation formulas. Of course, using the representation formulas to get such information would be overkill, because they can be obtained by brute force, i.e., by solving directly the equation

$$\boldsymbol{Q}^{\otimes r}\boldsymbol{H} = \boldsymbol{H}, \qquad \text{if } \boldsymbol{H} \text{ is a material tensor,} \tag{6.1}$$

or the equation

$$(\det \boldsymbol{Q})\,\boldsymbol{Q}^{\otimes r}\boldsymbol{H} = \boldsymbol{H}, \qquad \text{if } \boldsymbol{H} \text{ is a material pseudotensor.} \tag{6.2}$$

On the other hand, obtaining the restrictions on $\boldsymbol{H}$ and the UMPs carried by it by using the representation formulas and then by brute force will serve as a check on the correctness of the representation formulas and of the restrictions on texture coefficients derived in Chapter 5.

In this Chapter we will study material tensors and pseudotensors in the space $[V^{\otimes 2}]^{\otimes 2}]$, i.e., the space of 4th-order tensors that enjoy the major and minor symmetries. A familiar example of material tensors in this space is the elasticity tensor. Pseudotensors in $[V^{\otimes 2}]^{\otimes 2}]$ are seldom studied. For a material tensor or pseudotensor $\boldsymbol{H}$ in $[V^{\otimes 2}]^{\otimes 2}]$, we will use representation formulas (4.93), (4.94) and the restrictions on texture coefficients derived in Chapter 5 to determine the number of UMPs in $\boldsymbol{H}$ and the restrictions on the components of $\boldsymbol{H}$ imposed by G_{cr} for the cases of $G_{\mathrm{cr}} = C_s$, D_{3h}, C_{4v}, and D_{2d}. We elect to work with Type III crystals because representation formula (4.94) will hold for pseudotensors in $[V^{\otimes 2}]^{\otimes 2}]$, an instance for which the ad hoc approach in classical texture analysis to treat Type III crystals as if they are their Type I Laue-class peer will not work. We select C_s, D_{3h}, C_{4v}, and D_{2d} from the 10 Type III cases, because they represent the four subcases of Type III crystals as distinguished by the generator containing inversion (see Table 6.1). We will check the correctness of the findings by solving (6.1) and (6.2) directly.

Table 6.1: Four subcases in Type III.

	Generator containing inversion ($\boldsymbol{IR}$)	Groups
Subcase I	$\boldsymbol{IR}(e_3, \pi)$	C_s
Subcase II	$\boldsymbol{IR}(e_3, \frac{\pi}{3})$	C_{3h}, D_{3h}
Subcase III	$\boldsymbol{IR}(e_2, \pi)$	C_{2v}, C_{3v}, C_{4v}, C_{6v}
Subcase IV	$\boldsymbol{IR}(e_3, \frac{\pi}{2})$	S_4, D_{2d}, T_d

6.1 Crystal symmetry C_s

The point group C_s has only two elements, namely, the identity $\boldsymbol{E}$ and $\boldsymbol{IR}(e_3, \pi)$. We will first apply the general representation formula to both material tensors and pseudotensors with even order and then work out the details for material tensors and pseudotensors in $[[V_c^{\otimes 2}]^{\otimes 2}]$.

6.1.1 Even-order tensor

As shown in Chapter 5, invariance under $\boldsymbol{IR}(e_3,\pi)$ implies $c_{mn}^{l,R/L} = c_{mn}^{l,L/R}$ when n is even and $c_{mn}^{l,R/L} = -c_{mn}^{l,L/R}$ when n is odd. It follows that $b_{mn}^{l} = c_{mn}^{l,R} + c_{mn}^{l,L} = 0$ when n is odd. The representation formula (4.112) becomes

$$\boldsymbol{H}(w) = \boldsymbol{H}(w^R, w^L) = \sum_{k\in J}\sum_{s=1}^{n_k}\sum_{n=\text{even}}\sum_{m=-k}^{k} \alpha_n^{k,s} b_{mn}^{k} \boldsymbol{H}_m^{k,s} \tag{6.3}$$

where a procedure to obtain the orthonormal basis tensors $\boldsymbol{H}_m^{k,s}$ is given explicitly by Man and Huang [20].

To match the notation in Man and Huang's paper [20], let $\mathbf{C}(w) = \boldsymbol{H}(w)$ as a 4th-order elasticity tensor in $[[V_c^{\otimes 2}]^{\otimes 2}]$, which decomposes into its irreducible parts under O(3) according to formula (3.35). For this particular instance, (6.3) assumes the form

$$\mathbf{C}(w) = \mathbf{C}_{\text{iso}} + \sum_{s=1}^{2}\sum_{n=0,\pm 2} \alpha_n^{2,s}\boldsymbol{\Psi}_{ns} + \sum_{n=0,\pm 2,\pm 4} \alpha_n^{4}\boldsymbol{\Phi}_n, \tag{6.4}$$

where $\mathbf{C}_{\text{iso}}$ is given in equations (132)–(133) in Man and Huang's paper [20] with λ, μ as 2 undetermined material parameters, $\boldsymbol{\Psi}_{ns} = \sum_{m=-2}^{2} b_{mn}^{2}\mathbf{H}_m^{2,s}$, $\boldsymbol{\Phi}_n = \sum_{m=-4}^{4} b_{mn}^{4}\mathbf{H}_m^{4}$. The corresponding orthonormal basis tensors $\boldsymbol{H}_m^{k,s}$ are given by Man and Huang [20] and are reproduced in Appendix 2 of this thesis.

Note that for aggregates of crystallites with crystal symmetry C_s, the elasticity tensor $\mathbf{C}(w)$ carries 13 undetermined material parameters, 11 out of which are the α's in (6.4).

For single crystal with symmetry C_s, we can apply the restrictions imposed by sample symmetry on texture coefficients and have $c_{mn}^{k,R/L} = c_{mn}^{k,L/R}$ when m is even and $c_{mn}^{k,R/L} = -c_{mn}^{k,L/R}$

when m is odd, which implies $b^k_{mn} = 0$ when m is odd. Thus (6.3) becomes

$$\begin{aligned} \boldsymbol{H}(w) &= \boldsymbol{H}(w^R, w^L) \\ &= \sum_{k\in J}\sum_{s=1}^{n_k}\sum_{n=\text{even}}\sum_{m=-k}^{k} \alpha^{k,s}_{n,R} c^{k,R}_{mn} \boldsymbol{H}^{k,s}_m + \sum_{k\in J}\sum_{s=1}^{n_k}\sum_{n=\text{even}}\sum_{m=-k}^{k} \alpha^{k,s}_{n,L} c^{k,L}_{mn} \boldsymbol{H}^{k,s}_m \\ &= \sum_{k\in J}\sum_{s=1}^{n_k}\sum_{n,m=\text{even}} \alpha^{k,s}_{n} b^{k}_{mn} \boldsymbol{H}^{k,s}_m \end{aligned} \tag{6.5}$$

Using the formulas for $\boldsymbol{H}^{k,s}_m$ in $[[V_c^{\otimes 2}]^{\otimes 2}]$ with even m in Appendix 2, we obtain the following 6×6 matrix, which represents $\mathbf{C}(w) = \boldsymbol{H}(w)$ in the Voigt notation:

$$(c_{ij}) = \begin{pmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & c_{16} \\ & c_{22} & c_{23} & 0 & 0 & c_{26} \\ & & c_{33} & 0 & 0 & c_{36} \\ & & & c_{44} & c_{45} & 0 \\ & Sym & & & c_{55} & 0 \\ & & & & & c_{66} \end{pmatrix}, \tag{6.6}$$

where there are 13 undetermined material parameters.

On the other hand, the same 6×6 matrix is obtained by directly solving the matrix equation $\boldsymbol{Q}^{\otimes 4}\mathbf{C} = \mathbf{C}$ for $\boldsymbol{Q} \in C_s$ by hand and by using Maple.

6.1.2 Even-order pseudotensor

Again invariance under $\boldsymbol{IR}(e_3, \pi)$ implies $c^{l,R/L}_{mn} = c^{l,L/R}_{mn}$ when n is even and $c^{l,R/L}_{mn} = -c^{l,L/R}_{mn}$ when n is odd. Now we have $b^l_{mn} = c^{l,R}_{mn} - c^{l,L}_{mn} = 0$ when n is even. The representation formula (4.114) becomes

$$\boldsymbol{H}(w) = \boldsymbol{H}(w^R, w^L) = \sum_{k\in J}\sum_{s=1}^{n_k}\sum_{n=\text{odd}}\sum_{m=-k}^{k} \alpha^{k,s}_{n} b^{k}_{mn} \boldsymbol{H}^{k,s}_m \tag{6.7}$$

For a 4th-order pesudotensor in $[[V_c^{\otimes 2}]^{\otimes 2}]$, it follows that with $\mathbf{C}(w) = \boldsymbol{H}(w)$

$$\mathbf{C}(w) = \sum_{s=1}^{2} \sum_{n=\pm 1} \alpha_n^{2,s} \boldsymbol{\Psi}_{ns} + \sum_{n=\pm 1,\pm 3} \alpha_n^4 \boldsymbol{\Phi}_n. \tag{6.8}$$

Note that for aggregates of crystallites with $G_{\rm cr} = C_s$, the pseudotensor $\mathbf{C}(w)$ carries 8 undetermined material parameters, namely $\alpha_1^{2,1}, \alpha_{\bar{1}}^{2,1}, \alpha_1^{2,2}, \alpha_{\bar{1}}^{2,2}, \alpha_1^4, \alpha_{\bar{1}}^4, \alpha_3^4$, and $\alpha_{\bar{3}}^4$.

For single crystal with symmetry C_s, we have $b_{mn}^k = 0$ when m is odd. Then (6.7) reduces to the form

$$\boldsymbol{H}(w) = \boldsymbol{H}(w^R, w^L) = \sum_{k \in J} \sum_{s=1}^{n_k} \sum_{n,m=odd} \alpha_n^{k,s} b_{mn}^k \boldsymbol{H}_m^{k,s}. \tag{6.9}$$

On the one hand, using the formulas for the basis tensors $\boldsymbol{H}_m^{k,s}$ with odd m in Appendix 2, we obtain the 6×6 matrix (6.10) which represents $\mathbf{C}(w) = \boldsymbol{H}(w)$ in the Voigt notation. This matrix carries 8 independent undetermined parameters. On the other hand, this same matrix is obtained by directly solving the matrix equation $(\det \boldsymbol{Q})\, \boldsymbol{Q}^{\otimes 4}\mathbf{C} = \mathbf{C}$ for $\boldsymbol{Q} \in C_s$ by hand and by using Maple.

$$(c_{ij}) = \begin{pmatrix} 0 & 0 & 0 & c_{14} & c_{15} & 0 \\ & 0 & 0 & c_{24} & c_{25} & 0 \\ & & 0 & c_{34} & c_{35} & 0 \\ & & & 0 & 0 & c_{46} \\ & Sym & & & 0 & c_{56} \\ & & & & & 0 \end{pmatrix} \tag{6.10}$$

6.2 Crystal symmetry D_{3h}

For subcase II, we will use D_{3h} as an example. The calculations for crystal symmetry C_{3h} are similar. From chapter 5, the texture restrictions on crystal symmetry D_{3h} is given as follows:

(1) if $n = 6k$ for some integer k, then $c^{l,R}_{mn} = c^{l,L}_{mn}$ and we have $c^{l,R/L}_{mn} = (-1)^l c^{l,R/L}_{m\bar{n}}$;

(2) if $n = 6k + 3$ for some integer k, then $c^{l,R}_{mn} = -c^{l,L}_{mn}$ and $c^{l,R/L}_{mn} = (-1)^{l+1} c^{l,R/L}_{m\bar{n}}$.

6.2.1 Even-order tensor

Since C_s is a subgroup of D_{3h}, the representation formula should satisfy (6.3) with n even for non-zero terms b^l_{mn}. Together with the above texture restrictions, we have

$$\boldsymbol{H}(w) = \boldsymbol{H}(w^R, w^L) = \sum_{k\in J} \sum_{s=1}^{n_k} \sum_{n=\pm 0,\pm 6,\ldots} \sum_{m=-k}^{k} \alpha^{k,s}_n b^k_{mn} \boldsymbol{H}^{k,s}_m. \tag{6.11}$$

For elasticity tensor $\mathbf{C}(w)$ in $[[V_c^{\otimes 2}]^{\otimes 2}]$ by writing $\boldsymbol{H}(w) = \mathbf{C}(w)$, from (6.11) we then have

$$\mathbf{C}(w) = \mathbf{C}_{\text{iso}} + \sum_{s=1}^{2} \alpha^{2,s}_0 \mathbf{\Psi}_{0s} + \alpha^4_0 \mathbf{\Phi}_0, \tag{6.12}$$

where $\mathbf{\Psi}_{0s} = \sum_{m=-2}^{2} b^2_{m0} \mathbf{H}^{2,s}_m$, $\mathbf{\Phi}_0 = \sum_{m=-4}^{4} b^4_{m0} \mathbf{H}^4_m$.

We see that for aggregates of crystallites with crystal symmetry D_{3h}, the elasticity tensor $\mathbf{C}(w)$ carries 5 undetermined material parameters ($\lambda, \mu, \alpha^{2,1}_0, \alpha^{2,2}_0$ and α^4_0).

For single crystal with symmetry D_{3h}, we have $b^l_{mn} = 0$ unless $m = 6k, k \in \mathbb{Z}$. Thus (6.11) further reduces to

$$\boldsymbol{H}(w) = \boldsymbol{H}(w^R, w^L) = \sum_{k\in J} \sum_{s=1}^{n_k} \sum_{n,m=0,6,\ldots} \alpha^{k,s}_n b^k_{mn} \boldsymbol{H}^{k,s}_m. \tag{6.13}$$

In $[[V_c^{\otimes 2}]^{\otimes 2}]$, $b^l_{mn} = 0$ unless $m = 0$ because $m \leq 4$. The elasticity tensor $\mathbf{C}(w)$ in (6.12) then becomes

$$\mathbf{C}(w) = \mathbf{C}_{\text{iso}} + \sum_{s=1}^{2} \alpha^{2,s}_0 b^2_{00} \mathbf{H}^{2,s}_0 + \alpha^4_0 b^4_{00} \mathbf{H}^4_0 \tag{6.14}$$

Using the formulas for $\boldsymbol{H}_0^{k,s}$ with $k = 0, 2, 4$ and $s = 0, 1$ (See Appendix 2), we obtain the 6×6 matrix that represents $\mathbf{C}(w) = \boldsymbol{H}(w)$ in the Voigt notation:

$$(c_{ij}) = \begin{pmatrix} c_{12} + 2c_{66} & c_{12} & c_{13} & 0 & 0 & 0 \\ & c_{12} + 2c_{66} & c_{13} & 0 & 0 & 0 \\ & & c_{33} & 0 & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & Sym & & & c_{44} & 0 \\ & & & & & c_{66} \end{pmatrix} \tag{6.15}$$

We see that this matrix representation of $\mathbf{C}$ has 5 undetermined material parameters. Meanwhile, the same 6×6 matrix is also derived by directly solving the matrix equation $\boldsymbol{Q}^{\otimes 4}\mathbf{C} = \mathbf{C}$ for $\boldsymbol{Q} \in D_{3h}$ by hand and by using Maple.

6.2.2 Even-order pseudotensor

The representation formula should satisfy (6.7) since C_s is a subgroup of D_{3h}. With the restrictions on texture coefficient restrictions imposed by D_{3h}, we see that $b^l_{mn} = 0$ unless $n = 6k + 3$ with $k \in \mathbb{Z}$. The representation formula becomes

$$\boldsymbol{H}(w) = \boldsymbol{H}(w^R, w^L) = \sum_{k \in J} \sum_{s=1}^{n_k} \sum_{n=\pm 3, \pm 9, \ldots} \sum_{m=-k}^{k} \alpha_n^{k,s} b^k_{mn} \boldsymbol{H}_m^{k,s} \tag{6.16}$$

where $b^k_{mn} = c^{k,R}_{mn} - c^{k,L}_{mn}$ as in (4.112).

In $[[V_c^{\otimes 2}]^{\otimes 2}]$, it follows that

$$\mathbf{C}(w) = \sum_{n=\pm 3} \alpha_n^4 \sum_{m=-4}^{4} b^4_{mn} \boldsymbol{H}^4_m \tag{6.17}$$

From restrictions on texture coefficients imposed by D_{3h}, we also have $c^{l,R/L}_{mn} = (-1)^{l+1} c^{l,R/L}_{m\bar{n}}$ for $n = 6k + 3, k \in \mathbb{Z}$. Applying this in the space of $[[V_c^{\otimes 2}]^{\otimes 2}]$, we obtain $c^{R/L,4}_{m3} = -c^{R/L,4}_{m\bar{3}}$. It follows that $b^4_{m3} = c^{R,4}_{m3} - c^{L,4}_{m3} = -c^{R,4}_{m\bar{3}} + c^{L,4}_{m\bar{3}} = -(c^{R,4}_{m\bar{3}} - c^{L,4}_{m\bar{3}}) = -b^4_{m\bar{3}}$. Thus (6.17) becomes

$$\begin{aligned}\mathbf{C}(w) &= \sum_{n=\pm 3} \alpha^4_n \sum_{m=-4}^{4} b^4_{mn} \boldsymbol{H}^4_m = (\alpha^4_3 \sum_{m=-4}^{4} b^4_{m3} + \alpha^4_{\bar{3}} \sum_{m=-4}^{4} b^4_{m\bar{3}}) \boldsymbol{H}^4_m \\ &= (\alpha^4_3 \sum_{m=-4}^{4} b^4_{m3} - \alpha^4_{\bar{3}} \sum_{m=-4}^{4} b^4_{m3}) \boldsymbol{H}^4_m = \alpha_3 \sum_{m=-4}^{4} b^4_{m3} \boldsymbol{H}^4_m, \end{aligned} \tag{6.18}$$

where $\alpha_3 = \alpha^4_3 - \alpha^4_{\bar{3}}$.

For aggregates of crystallites with crystal symmetry D_{3h}, the pseudotensor $\mathbf{C}(w)$ just carries 1 undetermined material parameter α_3.

For single crystal with symmetry D_{3h}, we have $c^l_{mn} = 0$ unless $m = 6k + 3, k \in \mathbb{Z}$. In the space $[[V_c^{\otimes 2}]^{\otimes 2}]$, we obtain $b^4_{33} = -b^4_{\bar{3}3}$. It follows from (6.18) that

$$\mathbf{C}(w) = \alpha_3 \sum_{m=-4}^{4} b^4_{m3} \boldsymbol{H}^4_m = \alpha_3 (b^4_{33} \boldsymbol{H}^4_3 + b^4_{\bar{3}3} \boldsymbol{H}^4_{\bar{3}}) = \alpha_3 b^4_{33} (\boldsymbol{H}^4_3 - \boldsymbol{H}^4_{\bar{3}}) \tag{6.19}$$

The matrix elements in the 6×6 representation of $\mathbf{C}(w) = \boldsymbol{H}(w)$ are all zeros except possibly c_{14}, c_{24}, c_{15}, c_{25}, c_{46}, c_{56} and those on symmetric positions as in $\boldsymbol{H}^4_3$ and $\boldsymbol{H}^4_{\bar{3}}$ (See Appendix 2). Now note that $c_{14} = -c_{24} = c_{56} = \alpha_3 b^4_{33}[(\boldsymbol{H}^4_3)_{14} - (\boldsymbol{H}^4_{\bar{3}})_{14}] = \alpha_3 b^4_{33}(i - i) = 0$. Thus the non-zero elements are $c_{15} = -c_{25} = -c_{46} = \alpha_3 b^4_{33}(-1 - 1) = -2\alpha_3 b^4_{33}$. Hence $\mathbf{C}$ assumes the form

$$(c_{ij}) = \begin{pmatrix} 0 & 0 & 0 & 0 & -2\alpha_3 b^4_{33} & 0 \\ & 0 & 0 & 0 & 2\alpha_3 b^4_{33} & 0 \\ & & 0 & 0 & 0 & 0 \\ & & & 0 & 0 & 2\alpha_3 b^4_{33} \\ & Sym & & & 0 & 0 \\ & & & & & 0 \end{pmatrix} \tag{6.20}$$

This matrix has only one independent element (i.e., $c_{15} = -c_{25} = -c_{46}$). The same 6×6 matrix is obtained by directly solving the matrix equation $(\det \boldsymbol{Q})\, \boldsymbol{Q}^{\otimes 4} \mathbf{C} = \mathbf{C}$ for $\boldsymbol{Q} \in D_{3h}$.

6.3 Crystal symmetry C_{4v}

For groups C_{2v}, C_{3v}, C_{4v}, and C_{6v} in subcase III, we choose $C_{4v} = \langle \boldsymbol{R}(e_3, \frac{\pi}{2}), \boldsymbol{IR}(e_2, \pi)\rangle$ as an example. Restrictions on texture coefficients restrictions imposed by crystal symmetry C_{4v} derived in Chapter 5 show that

$$c^{l,R/L}_{mn} = \begin{cases} (-1)^l c^{l,L/R}_{m\bar{n}}, & \text{for } n = 4k, k \in \mathbb{Z}; \\ 0, & \text{else.} \end{cases} \tag{6.21}$$

Clearly, $b^l_{mn} = 0$ for both tensors and pseudotensors when n is not a multiple of 4. The representation formula (4.112) can then be reduced as

$$\boldsymbol{H}(w) = \boldsymbol{H}(w^R, w^L) = \sum_{k\in J} \sum_{s=1}^{n_k} \sum_{n=0,\pm4,\dots} \sum_{m=-k}^{k} \alpha^{k,s}_n b^k_{mn} \boldsymbol{H}^{k,s}_m, \tag{6.22}$$

where $b^k_{mn} = c^{k,R}_{mn} + c^{k,L}_{mn}$ for tensors and $b^k_{mn} = c^{k,R}_{mn} - c^{k,L}_{mn}$ for pseudotensors.

6.3.1 Even-order tensor

In Chapter 5, we have derived the restrictions $c^{k,R/L}_{mn} = (-1)^{l+n} c^{k,L/R}_{m\bar{n}}$, which are imposed by $\boldsymbol{IR}(e_2, \pi)$. Thus we have $b^k_{mn} = c^{k,R}_{mn} + c^{k,L}_{mn} = (-1)^{k+n} c^{k,L}_{m\bar{n}} + (-1)^{k+n} c^{k,R}_{m\bar{n}} = (-1)^{k+n} b^k_{m\bar{n}}$. In the space $[[V_c^{\otimes 2}]^{\otimes 2}]$, we have $k = 0, 2, 4$ and $n = -4, 0, 4$. Thus we obtain $b^4_{m4} = b^4_{m\bar{4}}$. By writing $\boldsymbol{H}(w)$ as $\mathbf{C}(w)$ for an elasticity tensor, (6.22) then can be simplified as

$$\begin{aligned} \mathbf{C}(w) &= \mathbf{C}_{\text{iso}} + \sum_{s=1}^{2} \alpha^{2,s}_0 \sum_{m=-2}^{2} b^2_{m0} \boldsymbol{H}^{2,s}_m + \sum_{n=0,\pm4} \alpha^4_n \sum_{m=-4}^{4} b^4_{mn} \boldsymbol{H}^4_m \\ &= \mathbf{C}_{\text{iso}} + \sum_{s=1}^{2} \alpha^{2,s}_0 \sum_{m=-2}^{2} b^2_{m0} \boldsymbol{H}^{2,s}_m + \alpha^4_0 \sum_{m=-4}^{4} b^4_{m0} \boldsymbol{H}^4_m + \alpha^4_4 \sum_{m=-4}^{4} b^4_{m4} \boldsymbol{H}^4_m + \alpha^4_{\bar{4}} \sum_{m=-4}^{4} b^4_{m\bar{4}} \boldsymbol{H}^4_m \\ &= \mathbf{C}_{\text{iso}} + \sum_{s=1}^{2} \alpha^{2,s}_0 \sum_{m=-2}^{2} b^2_{m0} \boldsymbol{H}^{2,s}_m + \sum_{n=0,4} \alpha^4_{n'} \sum_{m=-4}^{4} b^4_{mn} \boldsymbol{H}^4_m, \end{aligned} \tag{6.23}$$

where $\alpha^4_{0'} = \alpha^4_0$ and $\alpha^4_{4'} = \alpha^4_4 + \alpha^4_{\bar{4}}$.

We see that $\alpha^4_{4'}$ is a real number since α^4_4 and $\alpha^4_{\bar{4}}$ are complex conjugates [20]. Thus for aggregates of crystallites with crystal symmetry C_{4v}, the elasticity tensor $\mathbf{C}(w)$ carries 6 undetermined material parameters, namely $\lambda, \mu, \alpha^{2,1}_0, \alpha^{2,2}_0, \alpha^4_0$, and $\alpha^4_{4'}$.

For single crystal with symmetry C_{4v}, in $[[V_c^{\otimes 2}]^{\otimes 2}]$ we have $m = 4k, k \in \mathbb{Z}$ for non-zero terms in $\mathbf{C}$. Similarly, we obtain $b^4_{4n} = b^4_{\bar{4}n}$. By using the formulas for $\boldsymbol{H}^{k,s}_m$ with $m = 0, \pm 4$ (see Appendix 2), we obtain the following matrix expression for $\mathbf{C}$ in the Voigt notation:

$$(c_{ij}) = \begin{pmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & c_{16} \\ & c_{11} & c_{13} & 0 & 0 & -c_{16} \\ & & c_{33} & 0 & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & Sym & & & c_{44} & 0 \\ & & & & & c_{66} \end{pmatrix} \tag{6.24}$$

Moreover, $h_{16} = -h_{26}$ is non-zero only in $\boldsymbol{H}^4_4$ and $\boldsymbol{H}^4_{\bar{4}}$. However, $b^4_{4n}(\boldsymbol{H}^4_4)_{16} + b^4_{\bar{4}n}(\boldsymbol{H}^4_{\bar{4}})_{16} = b^4_{4n} \cdot (-i) + b^4_{\bar{4}n} \cdot i = 0$ implies $c_{16} = 0$ from (6.23). Similarly $c_{26} = -c_{16} = 0$. Therefore $\mathbf{C}$ can be expressed as follows in the Voigt notation with 6 independent elastic constants. Meanwhile, this matrix expression is obtained by directly solving the matrix equation $\boldsymbol{Q}^{\otimes 4}\mathbf{C} = \mathbf{C}$ for $\boldsymbol{Q} \in C_{4v}$ by hand and by using Maple.

$$(c_{ij}) = \begin{pmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ & c_{11} & c_{13} & 0 & 0 & 0 \\ & & c_{33} & 0 & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & Sym & & & c_{44} & 0 \\ & & & & & c_{66} \end{pmatrix} \tag{6.25}$$

6.3.2 Even-order pseudotensor

With $c^{k,R/L}_{mn} = (-1)^{k+n} c^{k,L/R}_{m\bar{n}}$ for pseudotensor, we have $b^k_{mn} = c^{k,R}_{mn} - c^{k,L}_{mn} = (-1)^{k+n} c^{k,L}_{m\bar{n}} - (-1)^{k+n} c^{k,R}_{m\bar{n}} = (-1)^{k+n}(-b^k_{m\bar{n}})$. In the space $[[V_c^{\otimes 2}]^{\otimes 2}]$, we have $k = 0, 2, 4$ and $n = -4, 0, 4$. It follows that $b^{k,s}_{m0} = -b^{k,s}_{m\bar{0}}$ for $k = 0, 2, 4$, and $b^4_{m4} = -b^4_{m\bar{4}}$. The former implies $b^{k,s}_{m0} = 0$. Then

(6.22) reduces to

$$
\begin{aligned}
\boldsymbol{H}(w) &= \sum_{n=\pm 4} \alpha_n^4 \sum_{m=-4}^{4} b_{mn}^4 \boldsymbol{H}_m^4 \\
&= \alpha_4^4 \sum_{m=-4}^{4} b_{m4}^4 \boldsymbol{H}_m^4 + \alpha_{\bar{4}}^4 \sum_{m=-4}^{4} b_{m\bar{4}}^4 \boldsymbol{H}_m^4 \\
&= (\alpha_4^4 - \alpha_{\bar{4}}^4) \sum_{m=-4}^{4} b_{m4}^4 \boldsymbol{H}_m^4 \\
&= \alpha_{4'}^4 \sum_{m=-4}^{4} b_{m4}^4 \boldsymbol{H}_m^4,
\end{aligned} \tag{6.26}
$$

where $\alpha_{4'}^4 = \alpha_4^4 - \alpha_{\bar{4}}^4$.

Note that for aggregates of crystallites with crystal symmetry C_{4v}, the pseudotensor $\boldsymbol{H}(w)$ carries just 1 undetermined material parameter $\alpha_{4'}^4$.

For single crystal with symmetry C_{4v}, we have $m = 4k, k \in \mathbb{Z}$ for non-zero terms in $\mathbf{C}(w) = \boldsymbol{H}(w)$ by analogue. Similarly we get $b_{44}^4 = -b_{\bar{4}4}^4$ and $b_{04}^4 = 0$. Thus (6.26) becomes

$$
\begin{aligned}
\mathbf{C}(w) &= \alpha_{4'}^4 \sum_{m=-4}^{4} b_{m4}^4 \boldsymbol{H}_m^4 \\
&= \alpha_{4'}^4 b_{44}^4 \boldsymbol{H}_4^4 + \alpha_{4'}^4 b_{\bar{4}4}^4 \boldsymbol{H}_{\bar{4}}^4 \\
&= \alpha_{4'}^4 b_{44}^4 (\boldsymbol{H}_4^4 - \boldsymbol{H}_{\bar{4}}^4)
\end{aligned} \tag{6.27}
$$

By observation, $\boldsymbol{H}_m = (h_{ij})$ with $m = \pm 4$ (see Appendix 2) have the following matrix expression in the Voigt notation:

$$
(h_{ij}) = \begin{pmatrix}
h_{11} & -h_{11} & 0 & 0 & 0 & h_{16} \\
 & h_{11} & 0 & 0 & 0 & -h_{16} \\
 & & 0 & 0 & 0 & 0 \\
 & & & 0 & 0 & 0 \\
 & Sym & & & 0 & 0 \\
 & & & & & h_{11}
\end{pmatrix}, \tag{6.28}
$$

where $h_{16} = -h_{26}$ is imaginary and $h_{11} = -h_{12} = h_{66}$ is real.

That $\overline{\boldsymbol{H}_4^4} = \boldsymbol{H}_4^4$ implies $(\boldsymbol{H}_4^4)_{ij} - (\boldsymbol{H}_4^4)_{ij} = 0$ if it is real. It follows that $c_{11} = c_{12} = c_{66} = 0$ in $\mathbf{C}(w)$ by (6.27). Therefore $\mathbf{C}(w)$ can be expressed as follows in the Voigt notation with one independent matrix entry. Similarly this 6×6 matrix expression is found by directly solving the matrix equation $(\det \boldsymbol{Q})\, \boldsymbol{Q}^{\otimes 4}\mathbf{C} = \mathbf{C}$ for $\boldsymbol{Q} \in C_{4v}$.

$$\mathbf{C}(w) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & c_{16} \\ & 0 & 0 & 0 & 0 & -c_{16} \\ & & 0 & 0 & 0 & 0 \\ & & & 0 & 0 & 0 \\ & Sym & & & 0 & 0 \\ & & & & & 0 \end{pmatrix} \tag{6.29}$$

6.4 Crystal symmetry D_{2d}

For groups in subcase IV (i.e., S_4, D_{2d} and T_d), we will discuss D_{2d} as an example, which is in the same Laue class as C_{4v} (see Section 6.3). As derived in Chapter 5, the restrictions imposed on non-trivial texture coefficients imposed by crystal symmetry D_{2d} are as follows:

(1) if $n = 0, \pm 4, \pm 8, \ldots$, then $c_{mn}^{k,R} = c_{mn}^{k,L}$ and $c_{mn}^{k,R/L} = (-1)^k c_{m\bar{n}}^{k,R/L}$;

(2) if $n = \pm 2, \pm 6, \pm 10, \ldots$, then $c_{mn}^{k,R} = -c_{mn}^{k,L}$ and $c_{mn}^{k,R/L} = (-1)^k c_{m\bar{n}}^{k,R/L}$.

For material tensors, we obtain $b_{mn}^k = c_{mn}^{k,R} + c_{mn}^{k,L} = 2c_{mn}^{k,R} = 2c_{mn}^{k,L}$ for $n = 4k$ with $k \in \mathbb{Z}$; Otherwise, $b_{mn}^k = 0$. And $b_{mn}^k = c_{mn}^{k,R} + c_{mn}^{k,L} = (-1)^k c_{m\bar{n}}^{k,R} + (-1)^k c_{m\bar{n}}^{k,R} = (-1)^k b_{m\bar{n}}^k$. Thus the representation formula (4.112) can be simplified as

$$\begin{aligned} \boldsymbol{H}(w) = \boldsymbol{H}(w^R, w^L) &= \sum_{k \in J} \sum_{s=1}^{n_k} \sum_{n=0,\pm 4,\ldots} \sum_{m=-k}^{k} \alpha_n^{k,s} b_{mn}^k \boldsymbol{H}_m^{k,s} \\ &= \sum_{k \in J} \sum_{s=1}^{n_k} \sum_{n=0,4,\ldots} \sum_{m=-k}^{k} \alpha_{n'}^{k,s} b_{mn}^k \boldsymbol{H}_m^{k,s}, \end{aligned} \tag{6.30}$$

where $b_{mn}^k = 2c_{mn}^{k,R} = 2c_{mn}^{k,L}$, $\alpha_{0'}^{k,s} = \alpha_0^{k,s}$ and $\alpha_{n'}^{k,s} = \alpha_n^{k,s} + (-1)^k \alpha_{\bar{n}}^{k,s}$.

For material pseudotensors, $b^k_{mn} = c^{k,R}_{mn} - c^{k,L}_{mn} = 2c^{k,R}_{mn} = -2c^{k,L}_{mn}$ for $n = 4k+2$ with $k \in \mathbb{Z}$; Otherwise, $b^k_{mn} = 0$. And again $b^k_{mn} = (-1)^k b^k_{m\bar{n}}$. It follows that the representation formula can be reduced as

$$\begin{aligned} \boldsymbol{H}(w) = \boldsymbol{H}(w^R, w^L) &= \sum_{k\in J} \sum_{s=1}^{n_k} \sum_{n=\pm 2,\pm 6,\ldots} \sum_{m=-k}^{k} \alpha^{k,s}_n b^k_{mn} \boldsymbol{H}^{k,s}_m \\ &= \sum_{k\in J} \sum_{s=1}^{n_k} \sum_{n=2,6,\ldots} \sum_{m=-k}^{k} \alpha^{k,s}_{n'} b^k_{mn} \boldsymbol{H}^{k,s}_m \end{aligned} \tag{6.31}$$

where $b^k_{mn} = 2c^{k,R}_{mn} = -2c^{k,L}_{mn}$ and $\alpha^{k,s}_{n'} = \alpha^{k,s}_n + (-1)^k \alpha^{k,s}_{\bar{n}}$.

6.4.1 Even-order tensor

In $[[V_c^{\otimes 2}]^{\otimes 2}]$, the values of k in (6.30) are restricted to $k = 0, 2, 4$. We obtain the following expression from (6.30) by writing $\mathbf{C}(w)$ for $\boldsymbol{H}(w)$ as an elasticity tensor:

$$\mathbf{C}(w) = \mathbf{C}_{\text{iso}} + \sum_{s=1}^{2} \alpha^{2,s}_0 \sum_{m=-2}^{2} b^2_{m0} \boldsymbol{H}^{2,s}_m + \sum_{n=0,4} \alpha^4_{n'} \sum_{m=-4}^{4} b^4_{mn} \boldsymbol{H}^4_m, \tag{6.32}$$

where $\alpha^4_{0'} = \alpha^4_0$ and $\alpha^4_{4'} = \alpha^4_4 + \alpha^4_{\bar{4}}$.

We see that for aggregates of crystallites with crystal symmetry D_{2d}, the elasticity tensor $\mathbf{C}(w)$ carries 6 undetermined material parameters ($\lambda, \mu, \alpha^{2,1}_0, \alpha^{2,2}_0, \alpha^4_{0'}$ and $\alpha^4_{4'}$).

For single crystal, we now have $b^k_{mn} = b^k_{\bar{m}n}$ and $m = 0, \pm 4$ for non-zero b^k_{mn}. By observation, $\boldsymbol{H}^{k,s}_m$ with $m = 0, \pm 4$ (see Appendix 2) all have the following matrix expression in Voigt notation:

$$(h_{ij}) = \begin{pmatrix} h_{11} & h_{12} & h_{13} & 0 & 0 & h_{16} \\ & h_{11} & h_{13} & 0 & 0 & -h_{16} \\ & & h_{33} & 0 & 0 & 0 \\ & & & h_{44} & 0 & 0 \\ & Sym & & & h_{44} & 0 \\ & & & & & h_{66} \end{pmatrix} \tag{6.33}$$

The matrix representation $\mathbf{C}(w)$ should also have this pattern by (6.32). Notice that $h_{16} = -h_{26} \neq 0$ only in $\boldsymbol{H}_4^4$ and $\boldsymbol{H}_{\bar{4}}^4$. Thus c_{16} in $\mathbf{C}(w)$ can be calculated as

$$c_{16} = \sum_{n=0,4} \alpha_{n'}^4 (b_{4n}^4 (\boldsymbol{H}_4^4)_{16} + b_{\bar{4}n}^4 (\boldsymbol{H}_{\bar{4}}^4)_{16}) = \sum_{n=0,4} \alpha_{n'}^4 (b_{4n}^4(-i) + b_{\bar{4}n}^4(i)) = 0. \tag{6.34}$$

Hence, we obtain the following matrix expression for $\boldsymbol{C}$ in the Voigt notation:

$$(c_{ij}) = \begin{pmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ & c_{11} & c_{13} & 0 & 0 & 0 \\ & & c_{33} & 0 & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & Sym & & & c_{44} & 0 \\ & & & & & c_{66} \end{pmatrix} \tag{6.35}$$

Therefore for the single crystal, $\mathbf{C}$ with symmetry D_{2d} has 6 independent undetermined parameters. And again, the same matrix expression (6.35) is found by directly solving the matrix equation $\boldsymbol{Q}^{\otimes 4}\mathbf{C} = \mathbf{C}$ for $\boldsymbol{Q} \in D_{2d}$ by hand and by using Maple.

6.4.2 Even-order pseudotensor

In the space $[[V_c^{\otimes 2}]^{\otimes 2}]$ with the values of k restricted to $0, 2, 4$, we see that $n = \pm 2$ for non-trivial b_{mn}^k. Now we obtain from (6.31) the following simplified representation formula:

$$\mathbf{C}(w) = \sum_{s=1}^{2} \alpha_{2'}^{2,s} \sum_{m=-2}^{2} b_{m2}^2 \boldsymbol{H}_m^{2,s} + \alpha_{2'}^4 \sum_{m=-4}^{4} b_{m2}^4 \boldsymbol{H}_m^4, \tag{6.36}$$

where $\alpha_{2'}^{2,s} = \alpha_2^{2,s} + \alpha_{\bar{2}}^{2,s}$ and $\alpha_{2'}^4 = \alpha_2^4 + \alpha_{\bar{2}}^4$.

Note that for aggregates of crystallites with crystal symmetry D_{2d}, the pseudotensor $\mathbf{C}(w)$ carries 3 undetermined material parameters ($\alpha_{2'}^{2,1}$, $\alpha_{2'}^{2,2}$ and $\alpha_{2'}^4$).

For the single crystal, in $[[V_c^{\otimes 2}]^{\otimes 2}]$ we have $m = \pm 2, k \in \mathbb{Z}$ for non-zero terms b^k_{mn} and $b^k_{mn} = b^k_{\bar{m}n}$. Then (6.36) can be further simplified as

$$\mathbf{C}(w) = \sum_{s=1}^{2} \alpha^{2,s}_{2'} b^2_{22} (\boldsymbol{H}^{2,s}_2 + \boldsymbol{H}^{2,s}_{\bar{2}}) + \alpha^4_{2'} b^4_{22} (\boldsymbol{H}^4_2 + \boldsymbol{H}^4_{\bar{2}}). \tag{6.37}$$

By observation, the matrix expressions $\boldsymbol{H}^{k,s}_m = (h_{ij})$ with $m = \pm 2$, $k = 2, 4$ and $s = 1, 2$ (see Appendix 2) all have the following form in the Voigt notation:

$$(h_{ij}) = \begin{pmatrix} h_{11} & 0 & h_{13} & 0 & 0 & h_{16} \\ & -h_{11} & -h_{13} & 0 & 0 & h_{16} \\ & & 0 & 0 & 0 & h_{36} \\ & & & h_{44} & h_{45} & 0 \\ & Sym & & & -h_{44} & 0 \\ & & & & & 0 \end{pmatrix}. \tag{6.38}$$

The matrix representation of $\mathbf{C}(w) = (c_{ij})$ should also have the same form because it is a linear combination of $\boldsymbol{H}^k_m$ with $m = \pm 2$, $k = 2, 4$. Notice that the entries h_{16}, h_{36} and h_{45} in all of these $\boldsymbol{H}^{k,s}_m$ are either zero or pure imaginary numbers. Together with $\overline{\boldsymbol{H}^k_m} = \boldsymbol{H}^k_{\bar{m}}$, we have $(\boldsymbol{H}^k_m)_{ij} + (\boldsymbol{H}^k_{\bar{m}})_{ij} = 0$ at these three positions. It follows that $c_{16} = c_{36} = c_{45} = 0$ in $\mathbf{C}(w)$ by (6.37). Together with (6.38), we obtain the following matrix expression in the Voigt notation for $\mathbf{C}(w)$:

$$\mathbf{C} = \begin{pmatrix} c_{11} & 0 & c_{13} & 0 & 0 & 0 \\ & -c_{11} & -c_{13} & 0 & 0 & 0 \\ & & 0 & 0 & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & Sym & & & -c_{44} & 0 \\ & & & & & 0 \end{pmatrix} \tag{6.39}$$

We see **C** with symmetry D_{2d} has 3 undetermined material parameters for the single crystal. The same matrix expression (6.39) is also obtained by directly solving the matrix equation $(\det \boldsymbol{Q})\, \boldsymbol{Q}^{\otimes 4}\mathbf{C} = \mathbf{C}$ for $\boldsymbol{Q} \in D_{2d}$.

6.5 Conclusion

In summary, Table 6.2 to Table 6.4 show the numbers of undetermined material parameters (UMP) in $[[V_c^{\otimes 2}]^{\otimes 2}]$ for aggregates of Type III crystallites and for aggregates with G_{cr} in Laue classes 2 and 8.

Table 6.2: Number of undetermined material parameters (UMP) in $[[V_c^{\otimes 2}]^{\otimes 2}]$ for aggregates of Type III crystallites.

G_{cr}	C_s	C_{2v}	S_4	C_{4v}	D_{2d}	C_{3v}	C_{3h}	D_{3h}	C_{6v}	T_d
UMP [r]	13	9	7	6	6	6	5	5	5	3
UMP [p]	8	4	6	1	3	1	2	1	0	0
G_p	C_1	C_2	C_2	C_4	D_2	C_3	C_3	D_3	C_6	T
UMP [r]	21	13	13	7	9	7	7	6	5	3
UMP [p]	21	13	13	7	9	7	7	6	5	3

$G_{cr} = G_p \cup \boldsymbol{IR}G_p$ for some $\boldsymbol{R} \in \mathrm{SO}(3)$ and $\boldsymbol{R} \notin G_p$; $[r]$ = (regular) material tensor; $[p]$ = material pseudotensor

Table 6.3: Number of undetermined material parameters (UMP) in $[[V_c^{\otimes 2}]^{\otimes 2}]$ for aggregates of Type III crystallites in the Laue Class 2.

G_{cr}	C_2 (Type I)	C_{2h} (Type II)	C_s (Type III)
UMP [r]	13	13	13
UMP [p]	13	0	8

Table 6.4: Number of undetermined material parameters (UMP) in $[[V_c^{\otimes 2}]^{\otimes 2}]$ for aggregates of Type III crystallites in the Laue Class 8.

G_{cr}	D_4 (Type I)	D_{4h} (Type II)	D_{2d} (Type III)	C_{4v} (Type III)
UMP [r]	6	6	6	6
UMP [p]	6	0	3	1

Appendix 1: Maple procedure

The following code is a procedure for Maple to compute the matrix elements of the Riemannian metric tensor g_{ij} in Section 2.2.3. To run this procedure, one must first load the package linalg.

```
Restart:
with(linalg):

R1:=matrix([[cos(psi), -sin(psi), 0], [sin(psi), cos(psi),0], [0, 0, 1]]):
R2:=matrix([[cos(theta), 0, sin(theta)], [0, 1,0], [-sin(theta), 0, cos(theta)]]):
R3:=matrix([[cos(phi), -sin(phi), 0], [sin(phi), cos(phi),0], [0, 0, 1]]):
E3:=matrix([[0,-1, 0], [1, 0,0], [0, 0, 0]]);
E2:=matrix([[0,0,1], [0, 0,0], [-1, 0, 0]]);
R:=multiply(R1,R2,R3);

g:=array(1..3,1..3):
g[1,1]:=simplify(1/2*trace(multiply(R1,E3,R2,R3,transpose(multiply(R1,E3,R2,R3))))):
g[1,2]:=simplify(1/2*trace(multiply(R1,E3,R2,R3,transpose(multiply(R1,R2,E2,R3))))):
g[1,3]:=simplify(1/2*trace(multiply(R1,E3,R2,R3,transpose(multiply(R1,R2,R3,E3))))):
g[2,2]:=simplify(1/2*trace(multiply(R1,R2,E2,R3,transpose(multiply(R1,R2,E2,R3))))):
g[2,3]:=simplify(1/2*trace(multiply(R1,R2,E2,R3,transpose(multiply(R1,R2,R3,E3))))):
g[3,3]:=simplify(1/2*trace(multiply(R1,R2,R3,E3,transpose(multiply(R1,R2,R3,E3))))):

for i from 2 to 3 do
for j from 1 to i-1 do
g[i,j]:=g[j,i]:
od: od:
print(g);
```

Appendix 2: Orthonormal basis tensors $\boldsymbol{H}_m^{k,s}$ in $[[V_c^2]^2]$

In Chapter 6 we use the 21 orthonormal irreducible basis tensors $\boldsymbol{H}_m^{k,s}$ ($k = 0, 2, 4; 1 \le s \le n_k; -k \le m \le k$) given by Man and Huang [20] for the tensor space $[[V_c^2]^2]$. These basis tensors are listed below. As those $\boldsymbol{H}_m^{k,s}$ with $m < 0$ are given in terms of their counterparts with $m > 0$ by $\boldsymbol{H}_m^{k,s} = (-1)^m \overline{\boldsymbol{H}_{\bar{m}}^{k,s}}$ (Also see Eq. $(4.95)_1$) , only the ones with $m \ge 0$ are displayed in Voigt notation [41]:

$$(\boldsymbol{H}_0^{0,1})_{ijkl} = \frac{\sqrt{5}}{15}[\delta_{ij}\delta_{kl} + (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})], \tag{40}$$

$$(\boldsymbol{H}_0^{0,2})_{ijkl} = \frac{1}{6}[2\delta_{ij}\delta_{kl} - (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})], \tag{41}$$

and,

$$\boldsymbol{H}_0^{2,1} = \frac{\sqrt{7}}{42}\begin{pmatrix} 6 & 2 & -1 & 0 & 0 & 0 \\ 2 & 6 & -1 & 0 & 0 & 0 \\ -1 & -1 & -12 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{pmatrix}, \tag{42}$$

$$\boldsymbol{H}_0^{2,2} = \frac{\sqrt{2}}{12}\begin{pmatrix} 0 & 4 & -2 & 0 & 0 & 0 \\ 4 & 0 & -2 & 0 & 0 & 0 \\ -2 & -2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -2 \end{pmatrix}, \tag{43}$$

$$\boldsymbol{H}_1^{2,1} = \frac{\sqrt{42}}{84}\begin{pmatrix} 0 & 0 & 0 & -i & 3 & 0 \\ 0 & 0 & 0 & -3i & 1 & 0 \\ 0 & 0 & 0 & -3i & 3 & 0 \\ -i & -3i & -3i & 0 & 0 & 1 \\ 3 & 1 & 3 & 0 & 0 & -i \\ 0 & 0 & 0 & 1 & -i & 0 \end{pmatrix}, \quad (44)$$

$$\boldsymbol{H}_1^{2,2} = \frac{\sqrt{3}}{12}\begin{pmatrix} 0 & 0 & 0 & -2i & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -2i & 0 & 0 & 0 & 0 & -1 \\ 0 & 2 & 0 & 0 & 0 & i \\ 0 & 0 & 0 & -1 & i & 0 \end{pmatrix} \quad (45)$$

$$\boldsymbol{H}_2^{2,1} = \frac{\sqrt{42}}{84}\begin{pmatrix} -6 & 0 & -1 & 0 & 0 & 3i \\ 0 & 6 & 1 & 0 & 0 & 3i \\ -1 & 1 & 0 & 0 & 0 & i \\ 0 & 0 & 0 & 1 & i & 0 \\ 0 & 0 & 0 & i & -1 & 0 \\ 3i & 3i & i & 0 & 0 & 0 \end{pmatrix}, \quad (46)$$

$$\boldsymbol{H}_2^{2,2} = \frac{\sqrt{3}}{12}\begin{pmatrix} 0 & 0 & -2 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ -2 & 2 & 0 & 0 & 0 & 2i \\ 0 & 0 & 0 & -1 & -i & 0 \\ 0 & 0 & 0 & -i & 1 & 0 \\ 0 & 0 & 2i & 0 & 0 & 0 \end{pmatrix}, \quad (47)$$

$$H_0^4 = \frac{\sqrt{70}}{140}\begin{pmatrix} 3 & 1 & -4 & 0 & 0 & 0 \\ 1 & 3 & -4 & 0 & 0 & 0 \\ -4 & -4 & 8 & 0 & 0 & 0 \\ 0 & 0 & 0 & -4 & 0 & 0 \\ 0 & 0 & 0 & 0 & -4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \tag{48}$$

$$H_1^4 = \frac{\sqrt{14}}{56}\begin{pmatrix} 0 & 0 & 0 & -i & 3 & 0 \\ 0 & 0 & 0 & -3i & 1 & 0 \\ 0 & 0 & 0 & 4i & -4 & 0 \\ -i & -3i & 4i & 0 & 0 & 1 \\ 3 & 1 & -4 & 0 & 0 & -i \\ 0 & 0 & 0 & 1 & -i & 0 \end{pmatrix}, \tag{49}$$

$$H_2^4 = \frac{\sqrt{7}}{28}\begin{pmatrix} -2 & 0 & 2 & 0 & 0 & i \\ 0 & 2 & -2 & 0 & 0 & i \\ 2 & -2 & 0 & 0 & 0 & -2i \\ 0 & 0 & 0 & -2 & -2i & 0 \\ 0 & 0 & 0 & -2i & 2 & 0 \\ i & i & -2i & 0 & 0 & 0 \end{pmatrix}, \tag{50}$$

$$H_3^4 = \frac{\sqrt{2}}{8}\begin{pmatrix} 0 & 0 & 0 & i & -1 & 0 \\ 0 & 0 & 0 & -i & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ i & -i & 0 & 0 & 0 & 1 \\ -1 & 1 & 0 & 0 & 0 & i \\ 0 & 0 & 0 & 1 & i & 0 \end{pmatrix}, \tag{51}$$

$$\boldsymbol{H}_4^4 = \frac{1}{4}\begin{pmatrix} 1 & -1 & 0 & 0 & 0 & -i \\ -1 & 1 & 0 & 0 & 0 & i \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -i & i & 0 & 0 & 0 & -1 \end{pmatrix}, \qquad \text{where } i = \sqrt{-1}. \tag{52}$$

Note that $s = 1$ when $n_k = 1$. We have suppressed the superscript s in $\boldsymbol{H}_m^{k,s}$ when $n_k = 1$, i.e., we write $\boldsymbol{H}_m^k$ for $\boldsymbol{H}_m^{k,1}$ when $n_k = 1$. Thus here $\boldsymbol{H}_m^4$ stands for $\boldsymbol{H}_m^{4,1}$ for each m.

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