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Identification of symmetry type of linear elastic stiffness tensor in an arbitrarily orientated coordinate system

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ABSTRACT

We develop a method through the mirror plane (MP) to identify the symmetry type of linear elastic stiffness tensor whose components are given with respect to an arbitrarily oriented coordinate system. The method is based on the irreducible decomposition of high-order tensor into a set of deviators and the multipole representation of a deviator into a scalar and a unit-vector set. Since a unit-vector depends on two Euler angles, we can illustrate the MP normals of the elastic tensor as zeros of a characteristic function on a unit disk and identify its symmetry immediately, which is clearer and simpler than the methods proposed before. Furthermore, by finding the common MPs of three unit-vector sets using Fortran recipes, we can also analytically recognize the symmetry type first and then recover the natural coordinate system associated with the linear elastic tensor. The structures of linear elastic stiffness tensors of real materials with all possible anisotropies are investigated in detail.

1. Introduction

Hooke's law connects the components of the strain and stress tensors, which under a given Cartesian coordinate system has the form of

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}, \tag{1}$$

where coefficients C_{ijkl} are the fourth-order elastic stiffness tensor satisfying the symmetries $C_{ijkl} = C_{jikl} = C_{klij}$, which arise from the symmetry of the stress and strain tensors and the requirement that the stress is derivable from a strain energy function. Here, and henceforth, all lower case Latin subscripts have the range from one to three, and the summation convention for repeated indices is implied.

The elastic stiffness tensor involved in (1) has at most 21 independent components. This number might be reduced if it exhibits material symmetries, which could arise from crystal structure, microstructure, etc. In the context of linear elasticity, the number of material symmetries has been proven to be eight (Huo and del Piero, 1991; Zheng and Boehler, 1994; He and Zheng, 1996; Forte and Vianello, 1996; Chadwick et al., 2001; Ting, 2003; Bóna et al., 2004). Namely a material is either isotropic or anisotropic, and that an anisotropic material is either triclinic (generally anisotropic), monoclinic, trigonal, orthogonal, tetragonal, cubic or transversely isotropic. There are two ways to express the symmetries of the linear elastic stiffness tensor or elastic tensor thereafter (Forte and Vianello, 1996; Chadwick et al., 2001): one is by the symmetry groups (Bóna et al., 2004), another is by the admitted sets of symmetry planes (Chadwick et al., 2001; Ting, 2003). Cowin and Mehrabadi (1995) showed that the operations associated with the symmetry groups of the elastic tensors, including the center of symmetry, the n-fold rotation axis and the n-fold inversion axis as well as the plane of (reflective) symmetry (namely mirror plane, abbreviated as MP in this paper) itself, can be developed from combinations of MPs, implying the equivalence of the two routes to analyze the symmetry of the elastic tensor (see Chadwick et al., 2001). Chadwick et al. (2001) argued that in general the restriction of the MP set is weaker than that of the symmetry group.

If the symmetry group of a material is not known *a priori*, then – except for the isotropic case, for which each coordinate system is a natural one – it is an inherent problem to recognize its symmetry type from the linear elastic tensor measured in an arbitrary coordinate system (Cowin and Mehrabadi, 1987; Cowin and Mehrabadi, 1995; Norris, 1989; Jaric, 1994). Cowin and Mehrabadi (1995) summarized that once the number and orientation of the normals to the symmetry planes of an elastic tensor are known, one can determine the symmetry type of the involved elastic material as follows. If there is no plane of symmetry, then the material belongs to triclinic. If there is one, it belongs to monoclinic. If there are three, then it is either orthorhombic or trigonal. If the three planes of symmetry are mutually perpendicular, it is orthorhombic; and if the three are coplanar, then it is trigonal. If there are five planes of

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symmetry, then the material belongs to tetragonal. If there are nine it belongs to cubic. If there are one plane of symmetry and a plane (same as the plane of symmetry) of isotropy, then the material is transversely isotropic. If every plane is a plane of symmetry, then the material is isotropic. However, the procedure suggested by Cowin and Mehrabadi (1995) for the determination of the number and orientation of symmetry planes is implicit and seems to depend on the nonzero of both C_{ijkk} and C_{ikkj}. Diner et al. (2010; see also François et al., 1998) developed a different method based on the concept of distance in the space of tensors, where, especially, the monoclinic and transversely isotropic distance functions are proposed because they depend only on two Euler angles and hence can be easily plotted. For instance, the monoclinic distance function (MDF)

$$d(\mathbf{C},\mathcal{L}^{mono}) = 4\left(C_{1113}^2 + C_{1123}^2 + C_{2213}^2 + C_{2223}^2 + C_{3313}^2 + C_{3323}^2 + 2C_{1223}^2 + 2C_{1213}^2\right) \tag{2}$$

vanishes if and only if the axis $\mathbf{e}_3$ is normal to one of the symmetry planes of the elastic tensor $\mathbf{C}$. Actually, the essence of an effective distance function is based on its ability to identify the MPs, and the concept of distance or proximity, as opposed to belonging, does not meet the spirit of the symmetry classification of elastic materials. Thus in the plot of MDF, only the observed number and location of the zeros will be helpful in the identification of the symmetry type. The MDF method must work through plotting, and its accuracy will be heavily intervened by the huge difference of elastic modulus for different materials even though their symmetries of elastic tensors are the same, which will result in a sharp variation in the distance function around the zero, and by the fact that usually there are more local minimums than zeros.

The objective of this paper is to present a novel method, from a different point of view and independent of the modulus, to recognize the MPs of the elastic tensors and also recover the corresponding natural coordinate system. We first decompose the elastic tensor into its irreducible parts, which in general include two isotropic terms defined by the Lamé coefficients λ and μ, and three anisotropic terms coming from two second-order deviators and a fourth-order deviator (Zou et al., 2001). we then represent every deviator with a scalar module and a set of unit vectors called the multipoles of the deviator (Zou and Zheng, 2003). The relevant geometric picture of the latter concept, 'bouquets of space directions', can be found in Backus (1970), which was further developed by Baerheim (1993, 1998) to classify the symmetry of the elastic tensor. The separations of tensor characteristic from the scalar modulus allow us to precisely recognize the MPs from three sets of unit vectors. In this way, we can, from the elastic tensor, define the indicator function relying on two Euler angles and plot it on a unit disk where the zeros of the function indicate the MP normals of the elastic tensor. Further, we develop an analytical procedure to determine all the MPs of the three unit-vector sets and find the rotation transformation back to the natural coordinate system of the elastic material.

The paper is constructed as follows. In Section 2, some basic concepts about the elastic tensor, such as its irreducible decomposition and multipole representation are elucidated. The class description of symmetry of the elastic tensor is presented based on the patterns of the corresponding unit-vector sets. In Section 3, we first introduce a characteristic function and plot it to recognize the MPs of the elastic tensor. A series of examples with all possible elastic anisotropies are illustrated, and some discussions are given. Then we propose an analytical procedure capable of judging the symmetry type of an elastic tensor from the analysis of its three unit-vector sets, and recovering the transformations back to the corresponding natural coordinate system. Finally, some concluding remarks are given in Section 4. The orthonormal base expansion of a deviator and the route from it to solve the unit-vector set and module of the deviator are given in the Appendix.

2. Structure and symmetry of an elastic tensor

2.1. Irreducible decomposition

With the scalar and vector being named as zeroth-order and first-order tensors, it is well-known that any higher-order tensor can be decomposed into some irreducible parts. For example, a general second-order tensor in three dimensions can be expressed by

$$T_{ij} = \alpha\delta_{ij} + \epsilon_{ijk}v_k + d_{ij}, \tag{3}$$

with the scalar α, the vector v_i and the second-order tracelessly symmetric tensor d_{ij} satisfying: $d_{ij} = d_{ji}, d_{kk} = 0$, where δ_{ij} is the second-order identity tensor and ϵ_{ijk} is the third-order permutation tensor. If T_{ij} is symmetric, such as the strain and stress tensors, the second term on the right hand side of (3) vanishes. A traceless and symmetric tensor is referred to as a deviator (deviatoric tensor). Especially, the scalar and vector are recognized as deviators of zeroth-order and first-order respectively. An irreducible tensor belongs to an irreducible and invariant subspace of the tensor space, and can be proved to be a combination of a deviator with an isotropic tensor made of some identity tensors or a half isotropic tensor made of some identity tensors and a permutation tensor. It is well known (cf. Backus, 1970; Cowin, 1989; Baerheim, 1993; Zou et al., 2001) that the irreducible decomposition of a linear elastic stiffness tensor has the form of

$$\begin{aligned} C_{ijkl} = {} & \lambda\delta_{ij}\delta_{kl} + \mu\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) + \delta_{ij}d_{kl}^1 + \delta_{kl}d_{ij}^1 \\ & + \left(\delta_{ik}d_{jl}^2 + \delta_{il}d_{jk}^2 + \delta_{jk}d_{il}^2 + \delta_{jl}d_{ik}^2\right) + D_{ijkl}, \end{aligned} \tag{4}$$

with two scalars λ and μ, called Lamé coefficients, two second-order deviators d_{ij}^1 and d_{ij}^2, and a fourth-order deviator D_{ijkl}. Multiplying one or two δ_{ij} for contraction, one can obtain the reciprocal representation as

$$\lambda = \frac{1}{15}(2C_{iikk} - C_{ikik}), \quad \mu = \frac{1}{30}(3C_{ikik} - C_{iikk}), \tag{5}$$

$$d_{ij}^1 = \frac{5}{7}\left(C_{kkij} - \frac{1}{3}C_{kkll}\delta_{ij}\right) - \frac{4}{7}\left(C_{kikj} - \frac{1}{3}C_{klkl}\delta_{ij}\right), \tag{6}$$

$$d_{ij}^2 = \frac{3}{7}\left(C_{kikj} - \frac{1}{3}C_{klkl}\delta_{ij}\right) - \frac{2}{7}\left(C_{kkij} - \frac{1}{3}C_{kkll}\delta_{ij}\right), \tag{7}$$

whereas the fourth-order deviator D_{ijkl} is determined.

Voigt (see Cowin and Mehrabadi, 1995) employed a matrix notation for the Hooke's law. In this notation, two symmetric indices in three dimensions are replaced by an index in six dimensions, say

$$11 \to 1; 22 \to 2; 33 \to 3; 23 \to 4; 31 \to 5; 12 \to 6. \tag{8}$$

Thus, the stress–strain relation (1) can be written as

$$\begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{pmatrix} \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ 2\varepsilon_4 \\ 2\varepsilon_5 \\ 2\varepsilon_6 \end{pmatrix}. \tag{9}$$

It is easy to see that the transformation matrix C_{IJ} is symmetric and has at most 21 distinct components. In Voigt's notation, we obtain the expressions of the Lamé coefficients

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$$\begin{cases} \lambda = \frac{1}{15}(C_{11}+C_{22}+C_{33}+4C_{12}+4C_{23}+4C_{13}-2C_{44}-2C_{55}-2C_{66}), \\ \mu = \frac{1}{15}(C_{11}+C_{22}+C_{33}-C_{12}-C_{23}-C_{13}+3C_{44}+3C_{55}+3C_{66}); \end{cases} \tag{10}$$

two sets of five distinct components of the second-order deviators d^1_{ij}

$$\begin{cases} d^1_{11} = \frac{1}{21}(2C_{11}-C_{22}-C_{33}+5C_{12}-10C_{23}+5C_{13}+8C_{44}-4C_{55}-4C_{66}), \\ d^1_{22} = \frac{1}{21}(2C_{22}-C_{11}-C_{33}+5C_{12}+5C_{23}-10C_{13}+8C_{55}-4C_{44}-4C_{66}), \\ d^1_{12} = \frac{1}{7}(C_{16}+C_{26}+5C_{36}-4C_{45}), \quad d^1_{23} = \frac{1}{7}(C_{24}+C_{34}+5C_{14}-4C_{56}), \\ d^1_{13} = \frac{1}{7}(C_{15}+C_{35}+5C_{25}-4C_{46}) \end{cases} \tag{11}$$

and d^2_{ij}

$$\begin{cases} d^2_{11} = \frac{1}{21}(2C_{11}-C_{22}-C_{33}-2C_{12}+4C_{23}-2C_{13}-6C_{44}+3C_{55}+3C_{66}), \\ d^2_{22} = \frac{1}{21}(2C_{22}-C_{11}-C_{33}-2C_{12}-2C_{23}+4C_{13}-6C_{55}+3C_{44}+3C_{66}), \\ d^2_{12} = \frac{1}{7}(C_{16}+C_{26}-2C_{36}+3C_{45}), \quad d^2_{23} = \frac{1}{7}(C_{24}+C_{34}-2C_{14}+3C_{56}), \\ d^2_{13} = \frac{1}{7}(C_{15}+C_{35}-2C_{25}+3C_{46}) \end{cases} \tag{12}$$

and nine distinct components of the fourth-order deviator D_{ijkl}

$$\begin{cases} D_{1111} = \frac{1}{35}(8C_{11}+3C_{22}+3C_{33}-8C_{12}+2C_{23}-8C_{13}+4C_{44}-16C_{55}-16C_{66}), \\ D_{2222} = \frac{1}{35}(8C_{22}+3C_{11}+3C_{33}-8C_{12}+2C_{13}-8C_{23}+4C_{55}-16C_{44}-16C_{66}), \\ D_{1122} = \frac{1}{35}(C_{33}-4C_{11}-4C_{22}+9C_{12}-C_{13}-C_{23}+18C_{66}-2C_{44}-2C_{55}), \\ D_{1123} = \frac{1}{7}(2C_{14}-C_{24}-C_{34}+4C_{56}), \quad D_{1113} = \frac{1}{7}(4C_{15}-C_{25}-3C_{35}-2C_{46}), \\ D_{1112} = \frac{1}{7}(4C_{16}-C_{36}-3C_{26}-2C_{45}), \quad D_{2213} = \frac{1}{7}(2C_{25}-C_{15}-C_{35}+4C_{46}), \\ D_{2212} = \frac{1}{7}(4C_{26}-C_{36}-3C_{16}-2C_{45}), \quad D_{2223} = \frac{1}{7}(4C_{24}-C_{14}-3C_{34}-2C_{56}). \end{cases} \tag{13}$$

2.2. Multipole representation of a deviator and its symmetry pattern

Although the pth-order deviator with $2p+1$ independent components is much simpler than the generic pth-order tensor with 3^p components, the structure of a deviator of higher order is still complicated. The geometric picture of a deviator can go back to the multipole representation of an arbitrary spherical harmonics suggested by Maxwell (1881). Backus (1970) observed that a totally symmetric tensor is equivalent to a homogeneous polynomial, and used the so-called 'harmonic decomposition' to represent a pth-order homogeneous polynomial in terms of $[p/2]$ unique harmonic polynomials of orders $p, p-2, \cdots$, where each tensor corresponding to a harmonic polynomial is called the harmonic tensor. Zou and Zheng (2003) established the Maxwell's multipole representation to express a pth-order deviator as the traceless symmetric part of the tensor product of p unit vectors $\mathbf{n}_r$ $(r = 1, \cdots, p)$, which are called the multipoles of the deviator, multiplied by a scalar A, such that

$$\mathbf{D}^{(p)} = A\lfloor \mathbf{n}_1 \otimes \cdots \otimes \mathbf{n}_p \rfloor. \tag{14}$$

In establishing the representation (14) (Zou, 2000), the first author of this paper was actually enlightened by the exercise 1.10 in the textbook of Chadwick (1979), and reminded of the multipole idea of Maxwell (1881). During the publication of Zou and Zheng (2003), the first author was aware of the perfect coincidence of (14) with the image of bouquets of directions proposed by Backus (1970). However, as pointed out by Zou and Zheng (2003), Eq. (14) represent better the spirit of tensor theory, and furthermore it is very straightforward for applications.

For the elastic tensor (4), one needs eight unit vectors

$$\mathbf{n}_r = \mathbf{n}(\theta_r, \varphi_r) = \mathbf{e}_3 \cos\theta_r + (\mathbf{e}_1 \cos\varphi_r + \mathbf{e}_2 \sin\varphi_r)\sin\theta_r, \quad r = 1, \cdots, 8, \tag{15}$$

to express the three deviators as

$$\mathbf{d}^1 = A_1\lfloor \mathbf{n}_1 \otimes \mathbf{n}_2 \rfloor, \quad \mathbf{d}^2 = A_2\lfloor \mathbf{n}_3 \otimes \mathbf{n}_4 \rfloor, \\ \mathbf{D} = A_3\lfloor \mathbf{n}_5 \otimes \mathbf{n}_6 \otimes \mathbf{n}_7 \otimes \mathbf{n}_8 \rfloor, \tag{16}$$

where the three scalars $A_k (k = 1, 2, 3)$ could be positive if proper choice, which are in general not unique (between the unit vector and its corresponding antipodal). The multipole representation (14) means that for a pth-order deviator there are $2p$ angular variables from a set of p unit vectors besides a modular variable. According to Zou and Zheng (2003), the procedure to solve the set of p unit vectors and the module of a deviator is algebraic as detailed in the Appendix.

If the sign of the module A is allowed to be indefinite, one can construct the unit-vector set freely from the unit vectors and their corresponding antipodals. That is to say, it becomes unnecessary to distinguish a unit vector from its antipodal in the unit-vector set. In the rest of this paper, we call a unit vector as an *axis-direction* instead. The axis-direction set can be used to reveal the structure and symmetry of a deviator, while the scalar module tells whether the structure and symmetry exist or not.

In the context of linear elasticity, MP is a powerful concept in identifying the type of symmetry (cf. Cowin and Mehrabadi, 1995). Let $\mathbf{n}$ be the unit vector normal to a plane and $\mathbf{m}$ any vector perpendicular to $\mathbf{n}$, thus $\mathbf{m} \cdot \mathbf{n} = 0$ for all $\mathbf{m}$. Typically, by choosing two unit vectors $\mathbf{m}_1$ and $\mathbf{m}_2$ orthogonal to each other such that the set $\{\mathbf{m}_1, \mathbf{m}_2, \mathbf{n}\}$ forms a right-hand coordinate system, one can recognize $\mathbf{m}$ as

$$\mathbf{m}_\phi = \mathbf{m}_1 \cos\phi + \mathbf{m}_2 \sin\phi. \tag{17}$$

The orthogonal transformation $\mathbf{R}_\mathbf{n}$ defined by a MP with normal $\mathbf{n}$ has properties

$$\mathbf{R}_\mathbf{n}\mathbf{n} = -\mathbf{n}, \quad \mathbf{R}_\mathbf{n}\mathbf{m}_\phi = \mathbf{m}_\phi, \quad \forall\phi \in [0, 2\pi). \tag{18}$$

Similarly, the MP normal $\mathbf{n}$ of a pth-order tensor $\mathbf{T}^{(p)}$ appears if and only if the invariant relation

$$\mathbf{R}_\mathbf{n}^{\times p}\mathbf{T}^{(p)} = \mathbf{T}^{(p)} \tag{19}$$

holds, where $\mathbf{R}_\mathbf{n}^{\times p}$ indicates the Kronecker powers of $\mathbf{R}_\mathbf{n}$ (see Zheng and Spencer, 1993). A plane of isotropy is a plane of mirror symmetry in which every vector is itself a MP normal.

A scalar takes any plane as its MP and thus it is isotropic. A plane is recognized to be the MP of an axis-direction set if and only if the mirror of every axis-direction with respect to the plane belongs to the set too. It is easy to prove that under the MP transformation the axis-directions in the set are either unchanged or changed in pair(s). In other words, the axis-directions must lie on the MP, or in pair(s): (i) reflect to be their antipodals, (ii) reflect to each other or equivalently make the MP as their mid-separate surface.

The MP symmetries of second- and fourth-order deviators are described below (Zou, 2000). A second-order deviator with a set of two axis-directions has two types of MP symmetries: transverse isotropy when two axis-directions are the same, and orthogonal symmetry otherwise. A fourth-order deviator with a set of four axis-directions has seven types of MP symmetries, just as those of the elastic tensor, namely (For simplicity, the coplanar MP normals are assumed to lie on the $(\mathbf{e}_1, \mathbf{e}_2)$-surface, the single MP normal is set to be the $\mathbf{e}_3(\mathbf{e})$-axis):

- Transverse isotropy (TI) if all four axes are the same, say $\mathbf{n}_5 = \mathbf{n}_6 = \mathbf{n}_7 = \mathbf{n}_8 = \mathbf{e}$, with $1+\infty$ MPs whose normals are $\mathbf{e}$ and all unit vectors normal to it.
- Cubic symmetry if a coordinate system $\{\mathbf{m}_1, \mathbf{m}_2, \mathbf{n}\}$ can be found to express the set of four axis-directions as

$$\{\mathbf{n}_5,\mathbf{n}_6,\mathbf{n}_7,\mathbf{n}_8\} = \left\{\frac{\mathbf{n}+\mathbf{m}_1+\mathbf{m}_2}{\sqrt{3}},\frac{\mathbf{n}-\mathbf{m}_1+\mathbf{m}_2}{\sqrt{3}},\frac{\mathbf{n}+\mathbf{m}_1-\mathbf{m}_2}{\sqrt{3}},\frac{-\mathbf{n}+\mathbf{m}_1+\mathbf{m}_2}{\sqrt{3}}\right\}, \tag{20}$$

with nine MPs as those of a cube.

- Tetragonal symmetry if four axis-directions come from an axis rotation around a distinct axis at 90°, say

$$\{\mathbf{n}_5,\mathbf{n}_6,\mathbf{n}_7,\mathbf{n}_8\} = \left\{\mathbf{n}\left(\theta,\varphi+\frac{k\pi}{2}\right),k=0,1,2,3\right\}, \tag{21}$$

with five MPs whose four normals are coplanar at 45° lying on another MP.

- Trigonal symmetry if three axis-directions come from an axis rotation around the fourth axis-direction at 120°, say

$$\{\mathbf{n}_5,\mathbf{n}_6,\mathbf{n}_7,\mathbf{n}_8\} = \left\{\mathbf{e},\mathbf{n}\left(\theta,\varphi+\frac{2k\pi}{3}\right),k=0,1,2\right\}, \tag{22}$$

with three MPs whose normals are coplanar at 120°.

- Orthogonal symmetry if one can find that the MPs orthogonal to each other is three, with the axis-direction set made of the following three kinds of sets with one, two or four elements if the three coordinate surfaces are assumed to be the MPs:

$$\begin{cases} S_W = \{\mathbf{n}(\theta,\varphi),\mathbf{n}(\theta,\pi-\varphi),\mathbf{n}(\theta,\pi+\varphi),\mathbf{n}(\theta,2\pi-\varphi)\}; \\ S_U = \{\mathbf{n}(\frac{\pi}{2},\varphi),\mathbf{n}(\frac{\pi}{2},\pi-\varphi)\} \text{ or } \{\mathbf{n}(\theta,0),\mathbf{n}(\theta,\pi)\} \text{ or } \{\mathbf{n}(\theta,\frac{\pi}{2}),\mathbf{n}(\theta,\frac{3\pi}{2})\}; \\ S_V = \{\mathbf{e}\} \text{ or } \{\mathbf{e}_1\}\text{or}\{\mathbf{e}_2\}. \end{cases} \tag{23}$$

- Monoclinic symmetry if there is only one MP, with four axis-directions lying on a plane (namely the MP) in pair(s) or making the plane as their mid-separate surface in pair(s).
- Triclinic (general anisotropy) if the four axis-directions are arbitrary (without a MP).

The above patterns of MPs are invariant under the transformation of coordinate system. Especially, one can identify the symmetry types of the second- and fourth-order deviators by simply counting the number of MPs, except for the trigonal and orthogonal symmetries that have three MPs but remarkably different patterns. Further, the MPs of the elastic tensor can be recognized as the common part of MPs of the three axis sets $\{\mathbf{n}_1,\mathbf{n}_2\}$, $\{\mathbf{n}_3,\mathbf{n}_4\}$ and $\{\mathbf{n}_5,\mathbf{n}_6,\mathbf{n}_7,\mathbf{n}_8\}$, which are derived from the three deviators obtained in (4).

2.3. MPs of the elastic tensor

Besides its isotropic part, the elastic tensor consists of at most two second-order deviators and a fourth-order deviator. Thus, from the aforementioned analysis of MP symmetry, one can deduce the MPs of the elastic tensor. For instance, two second-order deviators may be combined to be triclinic, monoclinic, orthogonal and transversely isotropic, belonging to a symmetry sub-class of the fourth-order deviator taking the cubic symmetry out and degenerating the trigonal and tetragonal symmetries into the transverse isotropy. In summary, we can list in Table 1 the spans of scalar modulus and patterns of the axis-direction sets under all possible symmetry types, where the blank means arbitrary and the symbol '-' means insignificant.

Theoretically, the number of independent variables of an elastic tensor of certain symmetry type may change within a large range. For example, the generally anisotropic elastic material has at most 21 independent components in its linear stiffness tensor, but at least 9 variables if it consists of a fourth-order deviator only. It should be noticed that the conventional statistics on the independent components of the elastic tensor with higher symmetries is carried out under a given coordinate axis or system where two or three angular variables are specified. The whole independent variables including these omitted angular variables are listed in Table 2, where the Lamé coefficients are assumed to be always nonzero, and the modular variables and angular variables (in the parentheses) are counted separately.

3. Symmetry identification of an elastic tensor

3.1. Two kinds of modulus

The Frobenius norm of a pth-order deviator

$$\left\|\mathbf{D}^{(p)}\right\| = \sqrt{D_{i_i\cdots i_p}D_{i_i\cdots i_p}} = |A|\left\|\lfloor\mathbf{n}_1\otimes\cdots\otimes\mathbf{n}_p\rfloor\right\| \tag{24}$$

is invariant under any orthogonal transformation. But, it is indeed a product of two kinds of modulus, namely the scalar module A and the so-called phase module

$$B = \left\|\lfloor\mathbf{n}_1\otimes\cdots\otimes\mathbf{n}_p\rfloor\right\|. \tag{25}$$

The nonzero scalar module indicates the existence of the deviator, while the phase module never equals to zero which implies some pattern information of the axis-direction set $\{\mathbf{n}_1,\cdots,\mathbf{n}_p\}$. For instance, the phase part of a second-order deviator with axis-direction set $\{\mathbf{n}_1,\mathbf{n}_2\}$ takes the form

$$\lfloor\mathbf{n}_1\otimes\mathbf{n}_2\rfloor = \frac{1}{2}(\mathbf{n}_1\otimes\mathbf{n}_2+\mathbf{n}_2\otimes\mathbf{n}_1) - \frac{1}{3}\gamma_{12}\mathbf{1}, \tag{26}$$

with $\gamma_{12} = \mathbf{n}_1\cdot\mathbf{n}_2$. The corresponding phase module can be deduced as

$$B = \|\lfloor\mathbf{n}_1\otimes\mathbf{n}_2\rfloor\| = \sqrt{\frac{1}{2}+\frac{1}{6}\gamma_{12}^2} \in \left[\sqrt{\frac{1}{2}},\sqrt{\frac{2}{3}}\right] \approx [0.7071, 0.8165]. \tag{27}$$

The maximum of B indicates the TI symmetry, whilst other values indicate the orthogonal symmetry.

For the phase part of a fourth-order deviator with the axis-direction set $\{\mathbf{n}_1,\mathbf{n}_2,\mathbf{n}_3,\mathbf{n}_4\}$, the expression is complicated as given below

$$\begin{aligned}\lfloor\mathbf{n}_1\otimes\mathbf{n}_2\otimes\mathbf{n}_3\otimes\mathbf{n}_4\rfloor = {}& \frac{1}{24}\langle\mathbf{n}_1\otimes\mathbf{n}_2\otimes\mathbf{n}_3\otimes\mathbf{n}_4\rangle \\ & -\frac{1}{84}[\gamma_{12}\langle\mathbf{1}\otimes\mathbf{n}_3\otimes\mathbf{n}_4\rangle + \gamma_{13}\langle\mathbf{1}\otimes\mathbf{n}_2\otimes\mathbf{n}_4\rangle \\ & +\gamma_{14}\langle\mathbf{1}\otimes\mathbf{n}_2\otimes\mathbf{n}_3\rangle + \gamma_{23}\langle\mathbf{1}\otimes\mathbf{n}_1\otimes\mathbf{n}_4\rangle \\ & +\gamma_{24}\langle\mathbf{1}\otimes\mathbf{n}_1\otimes\mathbf{n}_3\rangle + \gamma_{34}\langle\mathbf{1}\otimes\mathbf{n}_1\otimes\mathbf{n}_2\rangle] \\ & +\frac{1}{105}(\gamma_{12}\gamma_{34}+\gamma_{13}\gamma_{24}+\gamma_{14}\gamma_{23})\langle\mathbf{1}\otimes\mathbf{1}\rangle,\end{aligned} \tag{28}$$

where the symbol $\langle\rangle$ denotes the symmetrization operator not divided by the number of terms. If the fourth-order deviator has the TI symmetry, the expression (28) can be simplified to be

$$\lfloor\mathbf{n}^{\otimes 4}\rfloor = \mathbf{n}^{\otimes 4} - \frac{1}{7}\langle\mathbf{1}\otimes\mathbf{n}^{\otimes 2}\rangle + \frac{1}{35}\langle\mathbf{1}\otimes\mathbf{1}\rangle, \tag{29}$$

which yields the phase module

$$B = \|\lfloor\mathbf{n}^{\otimes 4}\rfloor\| = \sqrt{\frac{8}{35}} \approx 0.4781. \tag{30}$$

In other situations, the phase module of (28) depends on the six cosines $\gamma_{ij}(1\leqslant i\neq j\leqslant 4)$ and it is difficult to derive its theoretical formula.

It is interesting to find that the phase module (29) gives the maximum, and that the minimum of B is about 0.2434 coming from the fourth-order deviator with the cubic symmetry. In view of these and more data listed in the last column B_3 in Table 3, we conclude that it is unsuitable to use the phase module as the symmetry indicator of a deviator.

Table 1
Symmetry types of elastic tensors.

C		$\{\lambda,\mu\}$	$\mathbf{d}^1$		$\mathbf{d}^2$		**D**	
Types	Number of MP normals		A_1	$\{\mathbf{n}_1,\mathbf{n}_2\}$	A_2	$\{\mathbf{n}_3,\mathbf{n}_4\}$	A_3	$\{\mathbf{n}_5,\mathbf{n}_6,\mathbf{n}_7,\mathbf{n}_8\}$
Triclinic	0							
Monoclinic	1		$a^1_{2,1}=0$		$a^2_{2,1}=0$		$a_{4,1}=a_{4,3}=0$	
Orthogonal	3(orthogonal)			from (23)		from (23)		from (23)
Trigonal	3(coplanar)			$\{\mathbf{e}\}$		$\{\mathbf{e}\}$	$\neq 0$	(22)
Tetragonal	5(4 coplanar)			$\{\mathbf{e}\}$		$\{\mathbf{e}\}$	$\neq 0$	(21)
Cubic	9		0	–	0	–	$\neq 0$	(20)
TI	∞^1+1			$\{\mathbf{e}\}$		$\{\mathbf{e}\}$		$\{\mathbf{e}\}$
Isotropic	∞^3	$\neq 0$	0	–	0	–	0	–

Table 2
Numbers of independent modular and angular variables in an elastic tensor.

Types	Isotropic	TI	Cubic	Tetragonal	Trigonal	Orthogonal	Monoclinic	Triclinic
Numbers	2(0)	3–5(2)	3(3)	3–5(3–4)	3–5(4)	3–5(4–7)	3–5(6–10)	3–5(8–16)

3.2. Identification via MP pattern

Since the pioneering research of Voigt in the 1880s (see Love, 1944), the elastic tensors of various materials have been measured. According to the method described above, the module variables of the elastic materials with different symmetries are calculated and listed in Table 3. The data of the elastic tensors are collected from Sutcliffe (1992); Pan (2002); Yang (2005). First of all, if the scalar modulus A_1, A_2 and A_3 are negligible with respect to the Lamé coefficients λ and μ, the elastic tensor should be identified to be isotropic; otherwise, the elastic tensor is anisotropic and the MP patterns of its three deviators can be used to determine which type of anisotropy it belongs, where the criterion is simply given by the second column in Table 1.

From the discussion presented above, if the axis-direction $\mathbf{n}(\theta,\varphi)$ is the MP normal of the elastic tensor, then some components in the orthonormal base expansions (see the Appendix) of its deviators, namely $a^k_{2,1}$ $(k=1,2)$ of second-order deviators $\mathbf{d}^k$ $(k=1,2)$, $a_{4,1}$ and $a_{4,3}$ of fourth-order deviator $\mathbf{D}$, must be zero in the new coordinate system with $\mathbf{n}(\theta,\varphi)$ as its $\mathbf{e}$-axis. So we can introduce the following characteristic function (CF)

$$C(\theta,\varphi)=\frac{2}{N}\left(\frac{1}{\left\|\mathbf{d}^1\right\|^2}\left|a^1_{2,1}\right|^2+\frac{1}{\left\|\mathbf{d}^2\right\|^2}\left|a^2_{2,1}\right|^2+\frac{1}{\|\mathbf{D}\|^2}|a_{4,1}|^2+\frac{1}{\|\mathbf{D}\|^2}|a_{4,3}|^2\right), \tag{31}$$

to identify the pattern of MPs on a unit sphere, where N is the number of nonzero scalar modulus. It is obvious that the CF (31) is independent of all scalar modulus λ,μ,A_1,A_2, and A_3, and its zeros on the unit sphere directly determine the MP normals. Another interesting property of CF (31) is that its permitted maximum equals to 1, which is reached when the $(\mathbf{e}_1,\mathbf{e}_2)$-plane is a plane of the mirror antisymmetry of the tensor under consideration. However, it is impossible to reach the permitted maximum for an elastic tensor because it has no mirror antisymmetry, which can be observed in the subsequent figures.

Due to the symmetry of center inversion, the entire information of $C(\theta,\varphi)$ in Eq. (31) can be shown in the upper hemisphere. Further through the mapping

$$x=e^{\imath\varphi}\tan\frac{\theta}{2}, \tag{32}$$

we can plot the image of $C(\theta,\varphi)$ on the unit disk. Some typical examples are numerically shown in Fig. 1(*a-g*), where the resolution is of one degree in the Euler angles θ and φ. We note that in general the number of zeros does not equal to the number of minimums. For instance, there are many minimum points in Fig. 1(a,b) but most of them are not zero point; in Fig.1(d), the central minimum point is not a zero point.

Comparing with the MDF (2), which can be plotted on the unit disk too, we find that the pattern of the CF in Eq. (31) is clearer and more meaningful. While the image of MDF depends on the modulus of the elastic tensor and varies for different materials, the image

Table 3
Module variables of linear elasticity materials (Unit of scalar modulus: 10^{10}Pa).

Materials names (Types)	$\{\lambda,\mu\}$		$\mathbf{d}^1$		$\mathbf{d}^2$		**D**	
	λ	μ	A_1	B_1	A_2	B_2	A_3	B_3
$CuSO_4{\cdot}5H_2O$ (Triclinic)	2.443	1.378	1.113	0.7426	0.2989	0.7091	4.990	0.2897
Gypsum (Monoclinic)	3.255	1.719	2.434	0.7082	0.7682	0.7479	14.19	0.2878
Topaz (Orthogonal)	9.166	11.58	3.834	0.7239	0.4757	0.7111	22.11	0.3017
Gallium (Orthogonal)	3.332	3.745	1.589	0.7287	0.7629	0.7722	6.665	0.2881
Left-hand Quartz (Trigonal)	0.6160	4.781	0.3883	0.8165	0.9256	0.8165	31.67	0.2446
α-Quartz (Trigonal)	0.6800	4.767	0.1414	0.8165	0.7686	0.8165	30.72	0.2445
Tourmaline (Trigonal)	4.380	8.913	1.029	0.8165	3.571	0.8165	21.24	0.2728
Pentaerythritol (Tetragonal)	−0.06	0.3767	0.3043	0.8165	0.1057	0.8165	0.3980	0.3103
Tin (Tetragonal)	3.994	1.914	1.868	0.8165	1.205	0.8165	11.14	0.2473
Indium (Tetragonal)	3.764	0.5923	0.3979	0.8165	0.2741	0.8165	5.461	0.2769
Copper (Cubic)	10.24	5.440	0	–	0	–	46.35	0.2434
Silicon (Cubic)	5.245	6.810	0	–	0	–	25.79	0.2434
GaAs (Cubic)	4.320	4.820	0	–	0	–	24.30	0.2434
Beryl (TI)	8.352	7.984	1.393	0.8165	0.5279	0.8165	11.18	0.4781
Cobalt (TI)	13.40	8.451	3.977	0.8165	2.703	0.8165	15.77	0.4781
Magnesium (TI)	2.403	1.734	0.2729	0.8165	0.1421	0.8165	1.240	0.4781
PZT-4 ceramic (TI)	7.567	2.747	0.3071	0.8165	0.4571	0.8165	0.3000	0.4781

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of CF is determined only by the phase parts of the deviators extracted from the elastic tensor, especially for the elastic tensors of cubic materials for which all images of the CFs are the same. Using the elastic tensor of the cubic material given in Diner et al. (2010), where the rotation of the non-natural coordinate system has Euler angles $(4.6^\circ, 21.86^\circ, 33.95^\circ)$, we illustrate the patterns of these two functions given in Eqs. (2) and (31) in Fig. 2(*a-d*). It is observed that in the angle resolution the spans of MDF and CF are, respectively, $[0, 6.60]$ and $[0, 0.7407]$ in the natural coordinate system; however after the rotation they become $[0.0456, 6.60]$ and $[3.530 \times 10^{-5}, 0.7407]$, respectively. Another example shown in Fig. 3(*a-d*) is the trigonal elastic material α-Quartz, where the arbitrary rotation from the natural coordinate system has Euler angles $(110.82^\circ, 36.21^\circ, 123.23^\circ)$, and the corresponding spans under the natural and non-natural coordinate systems are $[1.47 \times 10^{-6}, 6.92]$ and $[0.0363, 6.92]$ for MDF, $[0, 0.6776]$ and $[1.169 \times 10^{-5}, 0.6778]$ for CF.

From these examples, we find that the probing precision loses quickly when the zeros depart from the sampling grid points, especially for the MDF whose zeros look like singular points. As for the trigonal example, since there are minimum points other than the zeros, the strategy proposed by Diner et al. (2010) for determining the zeros does not work. Up to now, there is no explicit method for obtaining the MPs of the elastic tensor, or in other words, no existing method is analytically feasible. For any distance functions proposed to determine the symmetry type of the elastic tensor of a given material (cf. Diner et al., 2010; Gazis et al., 1963; Moakher and Norris, 2006), regardless of its validity, figure illustration and identification are unavoidable.

Actually, from the transformation relations $(49)_2$ and the characteristic function (31), we can derive four equations equivalent to the conditions of zero point. For instance, one condition from the components of the deviator $\mathbf{d}^1$ is

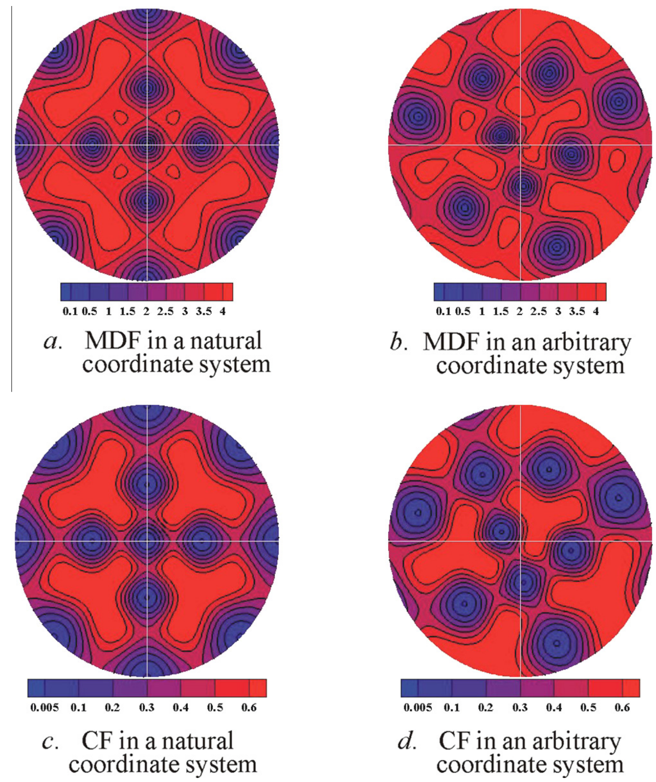

Fig. 2. Comparisons of the monoclinic distance function (MDF) and the characteristic function (CF) for the elastic tensor of the cubic material given by Diner et al. (2010), with rotation angles $(4.6^\circ, 21.86^\circ, 33.95^\circ)$ for the non-natural coordinate system.

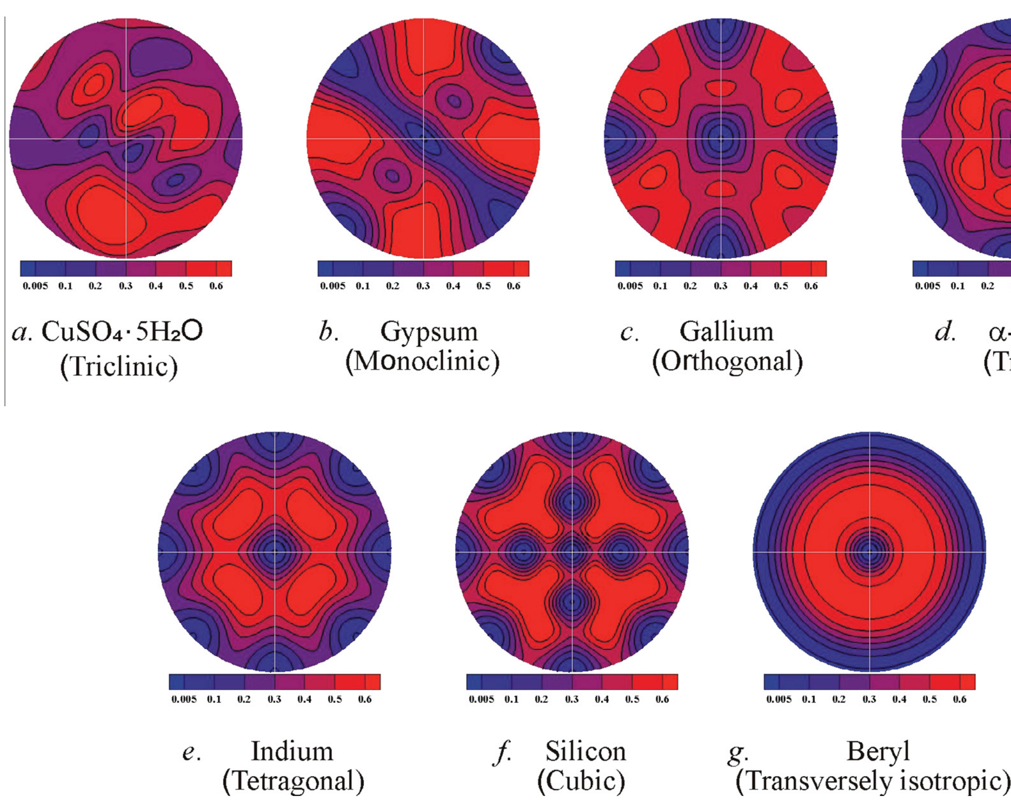

Fig. 1. Symmetry patterns of materials with various elastic anisotropies.

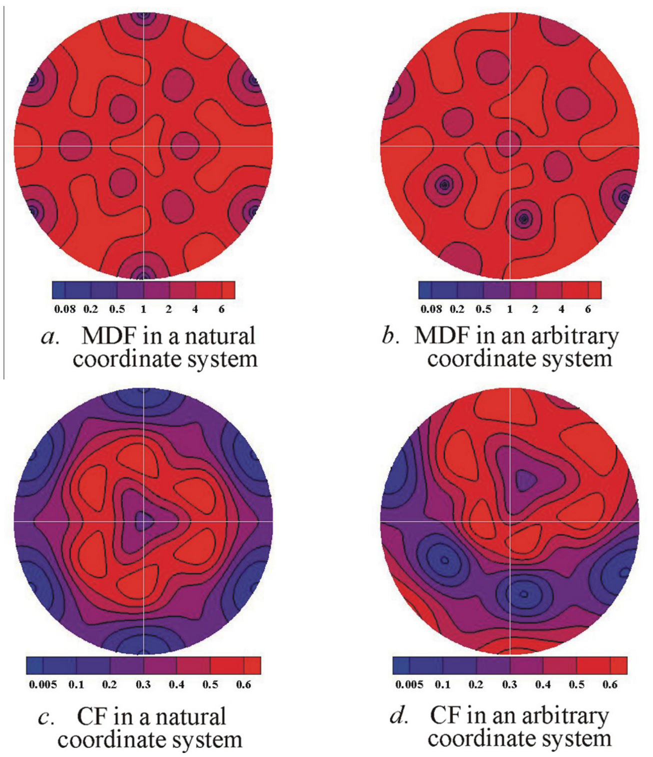

Fig. 3. Comparisons of the monoclinic distance function (MDF) and the characteristic function (CF) for the elastic tensor of the trigonal material α-Quartz, with arbitrary rotation angles $(110.82^\circ, 36.21^\circ, 123.23^\circ)$ for the non-natural coordinate system.

$$
\begin{aligned}
0 = a^{1\prime}_{2,1} &= \overline{D^{(2)}_{12}}\,\overline{a^1_{2,2}} - \overline{D^{(2)}_{11}}\,\overline{a^1_{2,1}} + \overline{D^{(2)}_{10}}\,a^1_{2,0} + \overline{D^{(2)}_{11}}\,a^1_{2,1} + \overline{D^{(2)}_{12}}\,a^1_{2,2} \\
&= -\overline{a^1_{2,2}}\sin\theta\frac{1-\cos\theta}{2}e^{-\imath 2\varphi} - \overline{a^1_{2,1}}(2\cos\theta+1)\frac{1-\cos\theta}{2}e^{-\imath\varphi} \\
&\quad - \sqrt{\frac{3}{2}}a^1_{2,0}\cos\theta\sin\theta + a^1_{2,1}(2\cos\theta-1)\frac{1+\cos\theta}{2}e^{\imath\varphi} + a^1_{2,2}\frac{1+\cos\theta}{2}\sin\theta e^{\imath 2\varphi},
\end{aligned}
$$

which is neither an algebraic equation of a single variable from two Euler angles, nor a equation solvable analytically.

3.3. Identification via multipole analysis

In this subsection, we develop an analytical method to determine the symmetry type of an elastic tensor of a given material based the three axis-direction sets.

First, in the natural coordinate system, the patterns of the axis-direction sets for the elastic tensors of different materials are presented in Fig. 4(*a*-*g*). Besides the sets of the two second-order deviators, which serve as backups in the identification process, the set pattern of the fourth-order deviator is completely fixed for TI and cubic symmetries, shape-unchanged for trigonal and tetragonal symmetries, alternative for orthogonal and monoclinic symmetries, and arbitrary for triclinic symmetry. Considering the appearance and relative movement of these multipoles, one can observe the evolving relation of the elastic tensor of the material from the low symmetry (triclinicity) to the high symmetry (isotropy) (see Chadwick et al., 2001).

Second, once the axis-direction sets $\{\mathbf{n}_1, \mathbf{n}_2\}, \{\mathbf{n}_3, \mathbf{n}_4\}$ and $\{\mathbf{n}_5, \mathbf{n}_6, \mathbf{n}_7, \mathbf{n}_8\}$ are solved from the components of the three deviators of an elastic tensor, we can then identify the symmetry type through their MPs and recover the transformation $\mathbf{R}(\phi, \theta, \varphi)$ with three Euler angles ϕ, θ, φ to its natural coordinate system of the tensor. The detailed procedure is as follows.

Denoting by MP[$\mathbf{T}$] the set of the MP normals of a tensor $\mathbf{T}$, then for the second-order deviator $\mathbf{d}^1$ we can obtain

$$
\mathrm{MP}\left[\mathbf{d}^1\right] = \begin{cases} \text{all directions(isotropic)}, & \text{if } A_1 = 0, \\ \{\mathbf{n}, \mathbf{m}_\phi, \phi \in [0, 2\pi)\}\text{(TI)}, & \text{if } A_1 \neq 0 \text{ and } \mathbf{n}_1 = \mathbf{n}_2 = \mathbf{n}, \\ \text{three principal directions(orthogonal)}, & \text{if } A_1 \neq 0 \text{ and } \mathbf{n}_1 \neq \mathbf{n}_2, \end{cases} \tag{33}
$$

where the principal directions are calculated by

$$
\mathbf{N}_1 = \frac{\mathbf{n}_1 + \mathbf{n}_2}{|\mathbf{n}_1 + \mathbf{n}_2|}, \quad \mathbf{N}_2 = \frac{\mathbf{n}_1 \times \mathbf{n}_2}{|\mathbf{n}_1 \times \mathbf{n}_2|}, \quad \mathbf{N}_3 = \mathbf{N}_1 \times \mathbf{N}_2. \tag{34}
$$

Similar expressions can be written for the other second-order deviator $\mathbf{d}^2$.

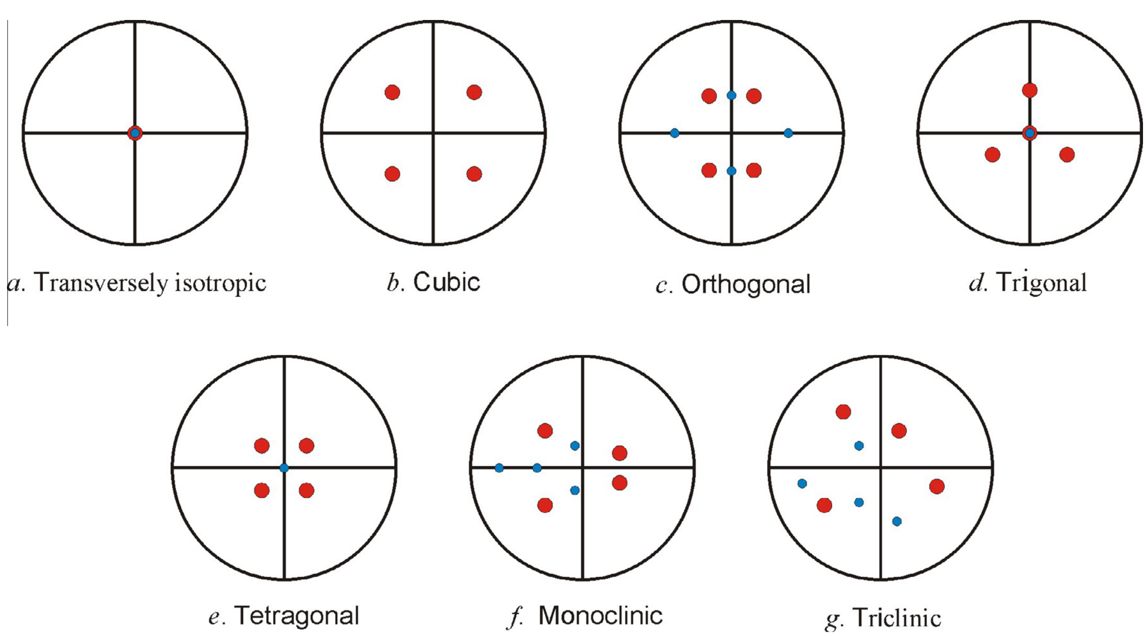

Fig. 4. Configurations of multipoles for the elastic tensor of different materials in their natural coordinate system (red bigger points from the fourth-order deviator, and blue smaller ones from the second-order deviators). The set patterns of the three deviators are completely fixed for TI and cubic symmetries, shape-unchanged for trigonal and tetragonal symmetries, and alternative for orthogonal and monoclinic. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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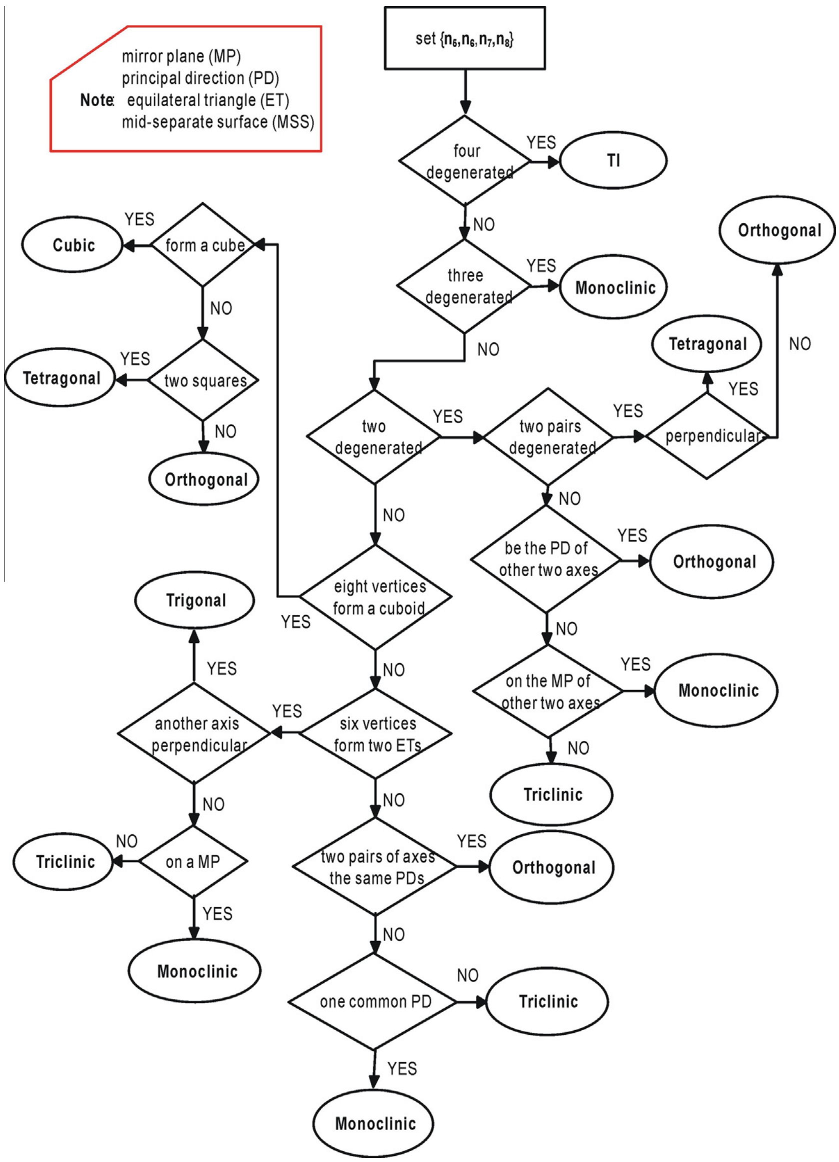

Fig. 5. Symmetry identification map of the fourth-order deviator **D**.

For the fourth-order deviator **D**, the recognition process of the MP normals, though being much complicated, can be carried out according to the flowchart shown in Fig. 5. The MP normals of the elastic tensor **C** is obtained by the intersection

$$\mathrm{MP}[\mathbf{C}] = \mathrm{MP}\left[\mathbf{d}^1\right] \cap \mathrm{MP}\left[\mathbf{d}^2\right] \cap \mathrm{MP}[\mathbf{D}] \tag{35}$$

and thus the symmetry type of the associated material can be identified from the second column in Table 1.

Finally, except for the triclinic (general) anisotropy and isotropy about which we have nothing to do, the transformation $\mathbf{R}(\phi, \theta, \varphi)$ to the natural coordinate system is found by

1. Assigning a direction $\mathbf{n}(\theta, \varphi)$ defined by two Euler angles θ, φ: if the symmetry is TI, it is the single MP normal $\mathbf{n}(\theta, \varphi)$; if the symmetry is cubic or orthogonal, the direction could be chosen to be one of the three MP normals perpendicular to each other; if the symmetry is trigonal or tetragonal, it is the direction normal to the coplanar MP normals; if the symmetry is monoclinic, the direction is the same as the MP normal.
2. determining the third Euler angle, or equivalently the direction $\mathbf{m}_1$ in the coordinate system $\{\mathbf{m}_1, \mathbf{m}_2, \mathbf{n}\}$. If the symmetry is TI or monoclinic, the third Euler angle is arbitrary and can be set to be zero; if the symmetry is cubic or orthogonal, $\mathbf{m}_1$ is the other one of the three MP normals perpendicular to each other. If the symmetry is trigonal or tetragonal, $\mathbf{m}_1$ can be chosen to be one of the coplanar MP normals.

The above procedure has been realized by us using Fortran codes, and testified with the elastic tensors of the materials listed in Table 3, after giving an arbitrary rotation transformation from the natural coordinate system. For example, the elastic tensor of the trigonal material α-Quartz is (Sutcliffe, 1992)

$$\begin{pmatrix} 8.76 & 0.60 & 1.33 & 0 & -1.73 & 0 \\ 0.60 & 8.76 & 1.33 & 0 & 1.73 & 0 \\ 1.33 & 1.33 & 10.68 & 0 & 0 & 0 \\ 0 & 0 & 0 & 5.72 & 0 & 1.73 \\ -1.73 & 1.73 & 0 & 0 & 5.72 & 0 \\ 0 & 0 & 0 & 1.73 & 0 & 4.08 \end{pmatrix}, \tag{36}$$

in its natural coordinate system. After an arbitrary rotation with Euler angles $(110.82^\circ, 36.21^\circ, 123.23^\circ)$, the corresponding elastic tensor becomes

$$C = \begin{pmatrix} 7.92 & 0.71 & 2.18 & -0.08 & -0.06 & -0.66 \\ 0.71 & 10.82 & -0.03 & 0.44 & -0.07 & 2.17 \\ 2.18 & -0.03 & 10.26 & 0.82 & 0.58 & -1.20 \\ -0.08 & 0.44 & 0.82 & 4.32 & -1.10 & 0.09 \\ -0.06 & -0.07 & 0.58 & -1.10 & 6.29 & 0.33 \\ -0.66 & 2.17 & -1.20 & 0.09 & 0.33 & 4.51 \end{pmatrix}. \quad (37)$$

Starting from the elastic tensor (37), we solve for the three axis-direction sets and find that their common MP normals are three coplanar axis-directions at 120° separation. Thus the material α-Quartz is judged to be a trigonal elastic material. The normal to the coplane

$$\mathbf{n}(\theta, \varphi) = -0.21\mathbf{e}_1 - 0.5522\mathbf{e}_2 - 0.8068\mathbf{e}_3 \quad (38)$$

is used as the direction to yield the two Euler angles θ, φ; and one of MP normals is chosen to be the $\mathbf{m}_2$-direction

$$\mathbf{m}_2 = 0.9171\mathbf{e}_1 - 0.3973\mathbf{e}_2 + 0.03326\mathbf{e}_3, \quad (39)$$

which defines the third Euler angle ϕ. Finally, we obtain the recovering Euler angles as

$$(\phi, \theta, \varphi) = (176.7724^\circ, 143.7857^\circ, -110.8217^\circ), \quad (40)$$

which define an inverse transformation, resulting in the following elastic tensor

$$\begin{pmatrix} 8.76 & 0.60 & 1.33 & 0 & 1.73 & 0 \\ 0.60 & 8.76 & 1.33 & 0 & -1.73 & 0 \\ 1.33 & 1.33 & 10.68 & 0 & 0 & 0 \\ 0 & 0 & 0 & 5.72 & 0 & -1.73 \\ 1.73 & -1.73 & 0 & 0 & 5.72 & 0 \\ 0 & 0 & 0 & -1.73 & 0 & 4.08 \end{pmatrix}. \quad (41)$$

in a natural coordinate system of the given material.

4. Concluding Remarks

A method to identify the symmetry type of the linear elastic stiffness tensor given in an arbitrary natural coordinate system is developed, utilizing the knowledge of the irreducible decomposition of the fourth-order elastic tensor and the multipole representations of deviators. Instead of the monoclinic distance function (MDF), we introduce a characteristic function (31) and plot it on a unit disk to identify the anisotropic types of the elastic tensor according to the zeros. Further, an analytical procedure is proposed to obtain the MPs of the given elastic tensor, which is the common part of the MPs of the three axis-direction sets derived from two second-order and a fourth-order deviators constituting the elastic tensor. The rotation transformation back to the natural coordinate system of the tensor is also presented, and various examples are analyzed to verify the accuracy of the proposed approach. Since we introduce the constructive representation (14) of a deviator and the concept of MP, our approach in identifying the symmetry of an elastic tensor is direct and more efficient as compared to previous methods (Backus, 1970; Baerheim, 1998).

We point out that, in reality, an elastic tensor of a given material could seem to be generally triclinic (without symmetries) due to experimental errors and/or the arbitrarily attached coordinate system. The accuracy of the parameter measurement may be estimated to ±3% for the tensor components and to be about ±5° for the angle (see François et al., 1998). These can be used as the thresholds in modulus selection, and as an error band to judge whether the axis-directions are parallel or normal to each other. However, it is impossible to find a simple function to define the distance between the elastic tensor measured experimentally and its nearest possible symmetry groups. For instance, the elastic tensor of the trigonal material α-Quartz, which looks like cubic in the plot of the MDF (see Fig. 3(a, b)), may become any one of the anisotropic types except for TI, if a disturbance larger than the threshold is admitted.

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Appendix A

A.1. Orthonormal base expansion of a deviator

According to Zou and Zheng (2003), the angular variables of unit vectors in (14) can be solved from an algebraic equation, and the module can be determined consequently. In order to use this method, we first introduce a set of complex orthonormal bases

$$\mathbf{E}_{p,r} = \sqrt{2^{p-r}\frac{(p+r)!(p-r)!}{(2p)!}} \sum_{s=0}^{[(p-r)/2]} \left(-\frac{1}{2}\right)^s \langle \mathbf{e}^{\otimes p-r-2s} \otimes \mathbf{w}^{\otimes r+s} \otimes \bar{\mathbf{w}}^{\otimes s} \rangle,$$
$$r = 0, 1, \cdots, p, \quad (42)$$

to expand a pth-order deviator $\mathbf{D}^{(p)}$ uniquely as

$$\mathbf{D}^{(p)} = a_{p,0}\mathbf{E}_{p,0} + \sum_{r=1}^{p} (a_{p,r}\mathbf{E}_{p,r} + \overline{a_{p,r}}\overline{\mathbf{E}_{p,r}}), \quad (43)$$

where $\mathbf{e} = \mathbf{e}_3, \mathbf{w} = \frac{1}{\sqrt{2}}(\mathbf{e}_1 + \imath\mathbf{e}_2), \imath = \sqrt{-1}$ is the unit imaginary number, the nth tensor power of vector () is denoted by $()^{\otimes n}$, $\bar{\mathbf{w}}$ and $\overline{\mathbf{E}_{p,r}}$ are the conjugates of $\mathbf{w}$ and $\mathbf{E}_{p,r}$ respectively. The operator $\langle\rangle$ in (42) represents the symmetrization without dividing by the number of summation terms, for example,

$$\langle \mathbf{e} \otimes \mathbf{w}^{\otimes 2} \rangle = \mathbf{e} \otimes \mathbf{w}^{\otimes 2} + \mathbf{w} \otimes \mathbf{e} \otimes \mathbf{w} + \mathbf{w}^{\otimes 2} \otimes \mathbf{e}. \quad (44)$$

Due to the orthogonality $\mathbf{E}_{p,r} \circ \overline{\mathbf{E}_{p,s}} = \delta_{rs}$, the expansion coefficients can be calculated from the complete scalar product

$$a_{p,r} = \overline{\mathbf{E}_{p,r}} \circ \mathbf{D}^{(p)}. \quad (45)$$

Making use of the notations

$$\mathbf{E}_{p,-r} = (-1)^r \overline{\mathbf{E}_{p,r}}, \quad a_{p,-r} = (-1)^r \overline{a_{p,r}}, \quad (46)$$

the expansion (43) can be rewritten in a compact form as

$$\mathbf{D}^{(p)} = \sum_{r=-p}^{p} a_{p,r}\mathbf{E}_{p,r}. \quad (47)$$

Under the rotation of the bases defined by three Euler angles

$$\mathbf{e}'_i = \mathbf{R}(\phi, \theta, \varphi)[\mathbf{e}_i] = \mathbf{R}_z(\phi)\mathbf{R}_y(\theta)\mathbf{R}_z(\varphi)[\mathbf{e}_i], \quad i = 1, 2, 3, \quad (48)$$

the coefficients of a pth-order deviator have the following transformation relations

$$a'_{p,r} = \sum_{s=-p}^{p} \overline{D_{rs}^{(p)}(\phi, \theta, \varphi)} a_{p,s} \quad (49)$$

due to the fact that

$$\mathbf{E}'_{p,r} = \mathbf{R}^{\times p}(\phi, \theta, \varphi)\left[\mathbf{E}_{p,r}\right] = \sum_{s=-p}^{p} D_{rs}^{(p)}(\phi, \theta, \varphi)\mathbf{E}_{p,s},$$

where the transformation matrix $D^{(p)}$ is given by

$$D_{rs}^{(p)}(\phi,\theta,\varphi)=\sum_{k=\max(0,s-r)}^{\min(p-r,p+s)}\frac{(-1)^k\sqrt{(p+r)!(p-r)!(p+s)!(p-s)!}}{k!(p-r-k)!(p+s-k)!(r-s+k)!}\, e^{-\imath r\phi}\left(\cos\frac{\theta}{2}\right)^{2p-r+s-2k}\left(-\sin\frac{\theta}{2}\right)^{r-s+2k}e^{-\imath s\varphi}. \qquad (50)$$

For instance, taking $p=1$, the transformation matrix can be written by

$$D^{(1)}(\phi,\theta,\varphi)=\begin{pmatrix} e^{-i\phi}\frac{1+\cos\theta}{2}e^{-i\varphi} & -e^{-i\phi}\frac{\sin\theta}{\sqrt{2}} & e^{-i\phi}\frac{1-\cos\theta}{2}e^{i\varphi}\\ \frac{\sin\theta}{\sqrt{2}}e^{-i\varphi} & \cos\theta & -\frac{\sin\theta}{\sqrt{2}}e^{i\varphi}\\ e^{i\phi}\frac{1-\cos\theta}{2}e^{-i\varphi} & e^{i\phi}\frac{\sin\theta}{\sqrt{2}} & e^{i\phi}\frac{1+\cos\theta}{2}e^{i\varphi}\end{pmatrix}. \qquad (51)$$

Applying this to the three deviators of an elastic tensor, we obtain the formulae of expansion coefficients as follows:

$$a_{2,0}^k=-\sqrt{\frac{3}{2}}\left(d_{11}^k+d_{22}^k\right),\quad a_{2,1}^k=d_{13}^k-\imath d_{23}^k,\quad a_{2,2}^k=\frac{1}{2}\left(d_{11}^k-d_{22}^k\right)-\imath d_{12}^k,\quad k=1,2; \qquad (52)$$

$$\begin{cases} a_{4,0}=\sqrt{\frac{35}{8}}(D_{1111}+D_{2222}+2D_{1122}),\\ a_{4,1}=\sqrt{\frac{7}{2}}[-D_{2213}-D_{1113}+\imath(D_{2223}+D_{1123})],\\ a_{4,2}=\frac{\sqrt{7}}{2}[D_{2222}-D_{1111}+2\imath(D_{2212}+D_{1112})],\\ a_{4,3}=\frac{1}{\sqrt{2}}[D_{1113}-3D_{2213}-\imath(3D_{1123}-D_{2223})],\\ a_{4,4}=\frac{1}{4}D_{1111}+\frac{1}{4}D_{2222}-\frac{3}{2}D_{1122}+\imath(D_{2212}-D_{1112}). \end{cases} \qquad (53)$$

A valuable property of this expansion is that it directly connects the components of a deviator with its structures. For example, the **e**-axis is the normal of the MP of an even-order deviator if and only if its base coefficients satisfy the condition $a_{p,2k+1}=0, k=0,1,\cdots,[p/2]$. Therefore, under the rotation $\mathbf{R}(0,\theta,\varphi)$ defined by two Euler angles θ and φ, one can make use of the zero points of the sum of modulus of $a_{2,1}^1, a_{2,1}^2, a_{4,1}$ and $a_{4,3}$ to identify the normals of the MPs, which is equivalent to the monoclinic distance function (2) given by Diner et al. (2010).

A.2. A.2 Calculations of angular and modular variables of deviators

Taking into account the property

$$\left(\mathbf{e}+\frac{x}{\sqrt{2}}\mathbf{w}-\frac{x^{-1}}{\sqrt{2}}\bar{\mathbf{w}}\right)\cdot\left(\mathbf{e}+\frac{x}{\sqrt{2}}\mathbf{w}-\frac{x^{-1}}{\sqrt{2}}\bar{\mathbf{w}}\right)=0, \qquad (54)$$

we further construct a tensorial polynomial

$$\mathbf{Z}_p=\left(\mathbf{e}+\frac{x}{\sqrt{2}}\mathbf{w}-\frac{x^{-1}}{\sqrt{2}}\bar{\mathbf{w}}\right)^{\otimes p}=\sum_{r=-p}^{p}\sqrt{\frac{2^{-p}(2p)!}{(p+r)!(p-r)!}}x^r\mathbf{E}_{p,r}, \qquad (55)$$

to derive the characteristic equations for the angular and modular variables of a pth-order deviator. Rewriting the unit vector, say (15) by

$$\mathbf{n}_r=\mathbf{e}\cos\theta_r+\frac{\mathbf{w}}{\sqrt{2}}e^{\imath\varphi_r}\sin\theta_r+\frac{\bar{\mathbf{w}}}{\sqrt{2}}e^{-\imath\varphi_r}\sin\theta_r,\quad r=1,\cdots,p \qquad (56)$$

and from the expressions (14) and (47) of a deviator, we obtain the complete inner product of $\mathbf{D}^{(p)}$ and $\mathbf{Z}_p$ as

$$\mathbf{D}^{(p)}\circ\mathbf{Z}_p=\sum_{r=-p}^{p}\sqrt{\frac{2^{-p}(2p)!}{(p+r)!(p-r)!}}(-1)^r a_{p,-r}x^r = A\prod_{r=1}^{p}\left(\cos\theta_r+\frac{xe^{\imath\varphi_r}}{2}\sin\theta_r-\frac{e^{-\imath\varphi_r}}{2x}\sin\theta_r\right). \qquad (57)$$

It is easy to find that if $a_{p,r}=0$ for $r=m+1,\cdots,p$, then there are $p-m$ unit vectors among the set identified as **e**, and other elements can be solved from the algebraic equation of x

$$a_{p,0}+\sum_{r=1}^{m}\sqrt{\frac{p!p!}{(p+r)!(p-r)!}}\left[x^r\overline{a_{p,r}}+(-1)^r x^{-r}a_{p,r}\right]=0. \qquad (58)$$

Obviously, x_r and $-\overline{x_r}^{-1}$ happen to be two roots of (58) at the same time, and further correspond to the unit vector $\mathbf{n}_r=\mathbf{n}(\theta_r,\varphi_r)$ and its antipodal by

$$x_r=e^{-\imath\varphi_r}\tan\frac{\theta_r}{2},\quad -\bar{x}_r^{-1}=e^{-\imath(\varphi_r+\pi\bmod 2\pi)}\tan\frac{\pi-\theta_r}{2}. \qquad (59)$$

By comparing the coefficient of the first term of x in (57), one can find that the scalar module A must be

$$A=\sqrt{2^{2m-p}\frac{(2p)!}{(p+m)!(p-m)!}}\overline{a_{p,m}}\prod_{r=1}^{m}e^{-\imath\varphi_r}\sec\theta_r. \qquad (60)$$

Thus, for the elastic tensor, through the characteristic Eq. (58), and using (11), (12), (13), (52) and (53), we are able to find all the angular and modular variables of the three involved deviators.

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