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Symmetry types of the piezoelectric tensor and their identification

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The third-order linear piezoelectricity tensor seems to be simpler than the fourth-order linear elasticity one, yet its total number of symmetry types is larger than the latter and the exact number is still inconclusive. In this paper, by means of the irreducible decomposition of the linear piezoelectricity tensor and the multipole representation of the corresponding four deviators, we conclude that there are 15 irreducible piezoelectric symmetry types, and thus further establish their characteristic web tree. By virtue of the notion of mirror symmetry and antisymmetry, we define three indicators with respect to two Euler angles and plot them on a unit disk in order to identify the symmetry type of a linear piezoelectricity tensor measured in an arbitrarily oriented coordinate system. Furthermore, an analytic procedure based on the solved axis-direction sets is also proposed to precisely determine the symmetry type of a linear piezoelectricity tensor and to trace the rotation transformation back to its natural coordinate system.

1. Introduction

In most smart materials (single crystals, ceramics, and thin films, etc.), an electric displacement is induced in response to an applied mechanical stress. This property is called the piezoelectric effect and a third-order matter tensor relates the induced electric displacement vector to the second-order stress tensor. This is expressed in the form

$$P_i = d_{ijk}\sigma_{jk}, \tag{1.1}$$

where P_i represents the electric displacement vector and σ_{jk} the stress tensor. The third-order piezoelectric

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matter tensor d_{ijk} has the symmetry $d_{ijk} = d_{ikj}$ due to the symmetry of the stress tensor. Here and henceforth, all lowercase Latin subscripts range from 1 to 3, and the summation convention for repeated subscripts or indices is implied.

The linear piezoelectricity tensor has a maximum of 18 distinct components. This number might be remarkably reduced if certain symmetries exist in the crystal structure, microstructure, etc. For instance, according to the definition on the piezoelectric effect, i.e. equation (1.1), all components of the piezoelectric tensor should vanish in materials possessing the centre of symmetry. It is further observed that, among all the three-dimensional material symmetry groups, namely the 41 compact-point groups comprising 32 crystal classes, seven Curie groups and two icosahedral groups [1–3], all the 15 centrosymmetric groups (i.e. the 11 crystal classes

$$\{C_i, C_{2h}, D_{2h}, C_{4h}, D_{4h}, S_6, D_{3d}, C_{6h}, D_{6h}, T_h, O_h\},$$

the three Curie groups $\{C_{\infty h}, D_{\infty h}, K_h\}$ and the icosahedral group I_h) will make the piezoelectricity property of materials null. Three other groups, namely crystal class O, Curie group K and icosahedral group I, also eliminate all piezoelectric components owing to their high symmetry restrictions. Thus, one needs to study at most 23 piezoelectric symmetry groups.

As for the remaining 23 piezoelectric symmetry groups, they could be further degenerated into certain independent symmetry types according to the invariance of the linear piezoelectricity tensor d_{ijk} under the symmetry transformation. While the number of d_{ijk} in different forms derived in a straightforward way was found to be 16 [1–6], Geymonat & Weller [7] claimed that 'the symmetry classes of piezoelectric tensors are found to be 14'. It is obvious that, up to now, the classification on linear piezoelectric symmetries is still contradictory and thus inconclusive. This motivates the present study. Therefore, in this paper, we would like to seek answers to the following three key questions: (i) The third-order piezoelectricity tensor is one order lower than the fourth-order elasticity tensor, and one would expect it to be simpler than the elasticity tensor; then why is the number of the irreducible symmetry types in the former larger than that in the latter which is 8 [8]? (ii) How many irreducible symmetry types are involved in a general linear piezoelectricity tensor? (iii) Is there any way to identify the type of a linear piezoelectricity tensor measured in an arbitrarily oriented coordinate system?

In order to answer these important questions, we make use of the irreducible decomposition and representation of high-order tensor [9,10], and further use for reference the recent approach on the identification of elasticity symmetry [11]. This paper is organized as follows. In §2, we decompose the linear piezoelectricity tensor into its irreducible parts, which in general consists of two vectors, a second-order deviator and a third-order deviator. We further express each deviator in terms of a scalar module and an axis-direction set. In §3, by virtue of the notion of mirror symmetry and antisymmetry ($\mathrm{MP}^{+/-}$, MP stands for mirror plane), we are able to clearly present the symmetry structures of a linear piezoelectricity tensor. This is achieved by analysing the associated deviators and by establishing the characteristic web tree of the symmetry groups. In §4, for the linear piezoelectricity coefficients measured in an arbitrarily oriented coordinate system, we define several indicators with respect to two Euler angles and plot them on a unit disk in order to recognize the $\mathrm{MP}^{+/-}$s of the piezoelectricity tensor. Furthermore, by solving the axis-direction sets, we also establish a procedure to analytically identify the symmetry types and eventually trace the rotation transformation back to its natural coordinate system. Finally, some concluding remarks are given in §5.

2. Structures of a linear piezoelectricity tensor

(a) Irreducible decomposition

A tensor is called a deviator if it is traceless and symmetric for any pair of indices of its Cartesian tensor components. For instance, any scalar and vector are, respectively, zeroth- and first-order

deviators, and a second-order deviator $\mathbf{D}^{(2)}$ (where the superscript '(2)' represents the order of the deviator) has components satisfying

$$D_{ij} = D_{ji}, \quad D_{kk} = 0. \tag{2.1}$$

It is well known from the theory of group representations that a tensor of any finite order can be decomposed into a sum of irreducible tensors, in which each irreducible tensor belongs to an irreducible and invariant subspace of the tensor space made of a deviator and two basic tensors (i.e. the identity tensor δ_{ij} and the permutation tensor ϵ_{ijk}). From Zou *et al.* [9], we know that the linear piezoelectricity tensor in general has the orthogonal irreducible decomposition

$$d_{ijk} = \delta_{jk}u_i + (\delta_{ij}v_k + \delta_{ik}v_j - \tfrac{2}{3}\delta_{jk}v_i) + (\epsilon_{iks}D_{sj} + \epsilon_{ijs}D_{sk}) + D_{ijk}, \tag{2.2}$$

where u_i and v_i are two vectors, D_{ij} and D_{ijk} are second- and third-order deviators, respectively. The decomposition is orthogonal because there is no coupling between different deviators in the square of Frobenius norm of $\mathbf{d}$ such that

$$\|\mathbf{d}\|^2 = 3\|\mathbf{u}\|^2 + \frac{20}{3}\|\mathbf{v}\|^2 + 6\|\mathbf{D}^{(2)}\|^2 + \|\mathbf{D}^{(3)}\|^2. \tag{2.3}$$

Multiplying δ_{ij} or ϵ_{ijk} on both sides of (2.3) for index contraction, one can find the following reciprocal representations for u_i, v_i, and D_{ij}

$$u_i = \tfrac{1}{3}d_{ikk}, \quad v_i = \tfrac{1}{10}(3d_{kki} - d_{ikk}) \tag{2.4}$$

and

$$D_{ij} = \tfrac{1}{6}(\epsilon_{imn}d_{mnj} + \epsilon_{jmn}d_{mni}), \tag{2.5}$$

Substituting equations (2.4) and (2.5) back to equation (2.2), we thus solve the third-order deviator D_{ijk}.

In practice, the two-index 'engineering' notation is often used. In terms of this notation, the two symmetric indices (i.e. j,k in equation (1.1)) ranging from 1 to 3 are replaced by a single index ranging from 1 to 6 as

$$11 \to 1; 22 \to 2; 33 \to 3; 23 \to 4; 31 \to 5; 12 \to 6. \tag{2.6}$$

Therefore, the matrix form of the electric displacement-stress relation (1.1) becomes

$$\begin{pmatrix} P_1 \\ P_2 \\ P_3 \end{pmatrix} = \begin{pmatrix} d_{11} & d_{12} & d_{13} & \sqrt{2}d_{14} & \sqrt{2}d_{15} & \sqrt{2}d_{16} \\ d_{21} & d_{22} & d_{23} & \sqrt{2}d_{24} & \sqrt{2}d_{25} & \sqrt{2}d_{26} \\ d_{31} & d_{32} & d_{33} & \sqrt{2}d_{34} & \sqrt{2}d_{35} & \sqrt{2}d_{36} \end{pmatrix} \begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sqrt{2}\sigma_4 \\ \sqrt{2}\sigma_5 \\ \sqrt{2}\sigma_6 \end{pmatrix}. \tag{2.7}$$

Also in terms of the engineering notation, the two vectors in equation (2.4) become

$$\left.\begin{aligned} u_i &= \tfrac{1}{3}(d_{i1} + d_{i2} + d_{i3}), i = 1, 2, 3; \\ v_1 &= \tfrac{1}{10}(3d_{26} + 3d_{35} + 2d_{11} - d_{12} - d_{13}), \\ v_2 &= \tfrac{1}{10}(3d_{16} + 3d_{34} + 2d_{22} - d_{23} - d_{21}), \\ v_3 &= \tfrac{1}{10}(3d_{15} + 3d_{24} + 2d_{33} - d_{31} - d_{32}); \end{aligned}\right\} \tag{2.8}$$

and the second-order deviator D_{ij} with five distinct components in equation (2.5) becomes

$$\left.\begin{aligned} &D_{11} = \tfrac{1}{3}(d_{25} - d_{36}), D_{22} = \tfrac{1}{3}(d_{36} - d_{14}), D_{12} = \tfrac{1}{6}(d_{24} - d_{32} + d_{31} - d_{15}), \\ &D_{23} = \tfrac{1}{6}(d_{35} - d_{13} + d_{12} - d_{26}), D_{13} = \tfrac{1}{6}(d_{23} - d_{34} + d_{16} - d_{21}). \end{aligned}\right\} \tag{2.9}$$

Finally, the third-order deviator D_{ijk} with seven distinct components has the following expressions

$$\left.\begin{aligned} &D_{111}=\tfrac{1}{5}(2d_{11}-d_{12}-d_{13}-2d_{26}-2d_{35}), \quad D_{222}=\tfrac{1}{5}(2d_{22}-d_{21}-d_{23}-2d_{16}-2d_{34}),\\ &D_{112}=\tfrac{1}{15}(8d_{16}-2d_{34}-3d_{22}-d_{23}+4d_{21}), \quad D_{113}=\tfrac{1}{15}(8d_{15}-2d_{24}-3d_{33}+4d_{31}-d_{32}),\\ &D_{221}=\tfrac{1}{15}(8d_{26}-2d_{35}-3d_{11}+4d_{12}-d_{13}), \quad D_{223}=\tfrac{1}{15}(8d_{24}-2d_{15}-3d_{33}-d_{31}+4d_{32})\\ \text{and}\quad &D_{123}=\tfrac{1}{3}(d_{36}+d_{14}+d_{25}). \end{aligned}\right\} \tag{2.10}$$

(b) Multipole representations

Following Zou and Zheng [10], a generic pth-order deviator has the Maxwell's multipole representation. In other words, the pth-order deviator $\mathbf{D}^{(p)}$ can be expressed as the tensor product of p unit vectors $\mathbf{n}_r (r=1,\ldots,p)$ (or called the multipoles of the deviator) multiplied by a scalar A,

$$\mathbf{D}^{(p)}=A\left\lfloor \mathbf{n}_1\otimes\cdots\otimes\mathbf{n}_p\right\rfloor, \tag{2.11}$$

where $\lfloor \boldsymbol{T}\rfloor$ denotes the traceless symmetric part of tensor $\boldsymbol{T}$. Thus, we need a total of seven unit vectors

$$\mathbf{n}_r=\mathbf{n}(\theta_r,\varphi_r)=\mathbf{e}_3\cos\theta_r+(\mathbf{e}_1\cos\varphi_r+\mathbf{e}_2\sin\varphi_r)\sin\theta_r, \quad r=1,\ldots,7, \tag{2.12}$$

to form four sets $\{\mathbf{n}_1\}$, $\{\mathbf{n}_2\}$, $\{\mathbf{n}_3,\mathbf{n}_4\}$ and $\{\mathbf{n}_5,\mathbf{n}_6,\mathbf{n}_7\}$ in order to represent the two vectors, a second- and a third-order deviator of the piezoelectricity tensor (2.2) as

$$\mathbf{u}=A_1\mathbf{n}_1, \mathbf{v}=A_2\mathbf{n}_2, \quad \mathbf{D}^{(2)}=A_3\left\lfloor \mathbf{n}_3\otimes\mathbf{n}_4\right\rfloor, \quad \mathbf{D}^{(3)}=A_4\left\lfloor \mathbf{n}_5\otimes\mathbf{n}_6\otimes\mathbf{n}_7\right\rfloor, \tag{2.13}$$

where the four scalars A_1 to A_4 can be positive if we properly choose the unit vectors and their antipodes in the corresponding unit-vector sets.

As shown in Zou *et al.* [11], the angular variables in (2.11) (without the scalar A) can be solved from the algebraic equation of x

$$a_{p,0}+\sum_{r=1}^{m}\sqrt{\frac{p!p!}{(p+r)!(p-r)!}}\left[x^r\bar{a}_{p,r}+(-1)^r x^{-r}a_{p,r}\right]=0, \tag{2.14}$$

where the overbar is used to denote the complex conjugation, and m indicates the largest second-index value r in the non-zero expansion coefficients $a_{p,r}$. In this equation, the variable x corresponds to a direction $\mathbf{n}(\theta,\varphi)$ by

$$x=\mathrm{e}^{-\mathrm{i}\varphi}\tan\frac{\theta}{2}, \tag{2.15}$$

with $\mathrm{i}=\sqrt{-1}$ being the unit imaginary number, and $a_{p,r}$ are the components of the deviator $\mathbf{D}^{(p)}$ in terms of the orthonormal bases

$$\mathbf{E}_{p,r}=\sqrt{2^{p-r}\binom{2p}{p+r}^{-1}}\sum_{s=0}^{[(p-r)/2]}\left(-\frac{1}{2}\right)^s\left\langle \mathbf{e}^{\otimes p-r-2s}\otimes\mathbf{w}^{\otimes r+s}\otimes\bar{\mathbf{w}}^{\otimes s}\right\rangle, \quad r=0,1,\ldots,p. \tag{2.16}$$

In other words, in terms of these orthonormal bases, we have [12,13]

$$\mathbf{D}^{(p)}=\sum_{r=-p}^{p}a_{p,r}\mathbf{E}_{p,r}, \quad a_{p,r}=\bar{\mathbf{E}}_{p,r}\circ\mathbf{D}^{(p)}, \tag{2.17}$$

due to the orthogonality $\mathbf{E}_{p,r}\circ\bar{\mathbf{E}}_{p,s}=\delta_{rs}$. Also in equation (2.16), $\mathbf{e}=\mathbf{e}_3$; $\mathbf{w}=\frac{1}{\sqrt{2}}(\mathbf{e}_1+\mathrm{i}\mathbf{e}_2)$; $\binom{2p}{p+r}=\frac{(2p)!}{(p+r)!(p-r)!}$ is the binomial coefficient; the pth tensor powers of a vector $\mathbf{e}$ is denoted by $\mathbf{e}^{\otimes p}$; the operator 'o' indicates the complete scalar product; and the operator '$\langle\cdot\rangle$' represents the

symmetrization operation without normalization by the total number of the terms involved. As an example for the operator $\langle\cdot\rangle$, we will have,

$$\left\langle \mathbf{e}\otimes\mathbf{w}^{\otimes 2}\right\rangle = \mathbf{e}\otimes\mathbf{w}^{\otimes 2} + \mathbf{w}\otimes\mathbf{e}\otimes\mathbf{w} + \mathbf{w}^{\otimes 2}\otimes\mathbf{e}. \tag{2.18}$$

We also point out, without loss of generality, that we have assumed $a_{p,m}\neq 0$ while in equation (2.17) $a_{p,r}=0(r=m+1,\ldots,p)$ with respect to the selected coordinate system. This means that there are $p-m$ unit vectors among the set $\{\mathbf{n}_r,(r=1,\ldots,p)\}$ taking to be $\mathbf{e}$ or $-\mathbf{e}$. Since x_r and $-\bar{x}_r^{-1}$ happen to be two roots of equation (2.14), corresponding to a unit vector $\mathbf{n}_r=\mathbf{n}(\theta_r,\varphi_r)$ and its antipode by

$$x_r = \mathrm{e}^{-\mathrm{i}\varphi_r}\tan\frac{\theta_r}{2},\quad -\bar{x}_r^{-1} = \mathrm{e}^{-\mathrm{i}(\varphi_r+\pi \bmod 2\pi)}\tan\frac{\pi-\theta_r}{2}, \tag{2.19}$$

the solution of equation (2.14) actually represents a set of *axis-directions*. Once the set of unit vectors of a deviator is given, the modular variable A can be calculated by the formula

$$A = \sqrt{2^{2m-p}\binom{2p}{p+m}}\,\bar{a}_{p,m}\prod_{r=1}^{m}\mathrm{e}^{-\mathrm{i}\varphi_r}\sec\theta_r. \tag{2.20}$$

This concludes our derivation where a generic pth-order deviator is expressed by the Maxwell's multipole representation. As for the two vectors, the second- and third-order deviators of the piezoelectricity tensor, the expansion components can be derived from (2.8)–(2.10) and $(2.17)_2$ as follows (superscripts u and v are used to distinguish the expansions for the two vectors $\mathbf{u}$ and $\mathbf{v}$):

$$\left.\begin{aligned} a^{\mathrm{u}}_{1,0} &= \tfrac{1}{3}(d_{31}+d_{32}+d_{33}),\\ a^{\mathrm{u}}_{1,1} &= \tfrac{1}{3\sqrt{2}}[(d_{11}+d_{12}+d_{13}) - i(d_{21}+d_{22}+d_{23})];\end{aligned}\right\} \tag{2.21}$$

$$\left.\begin{aligned} a^{\mathrm{v}}_{1,0} &= \tfrac{1}{10}(3d_{15}+3d_{24}+2d_{33}-d_{31}-d_{32}),\\ a^{\mathrm{v}}_{1,1} &= \tfrac{1}{10\sqrt{2}}[(3d_{26}+3d_{35}+2d_{11}-d_{12}-d_{13}) - i(3d_{16}+3d_{34}+2d_{22}-d_{23}-d_{21})],\end{aligned}\right\} \tag{2.22}$$

$$\left.\begin{aligned} &a_{2,0} = -\sqrt{\tfrac{1}{6}}(d_{25}-d_{14}), a_{2,1} = \tfrac{1}{6}[d_{23}-d_{34}+d_{16}-d_{21} - i(d_{35}-d_{13}+d_{12}-d_{26})],\\ &a_{2,2} = \tfrac{1}{6}[d_{25}+d_{14}-2d_{36} - i(d_{24}-d_{32}+d_{31}-d_{15})],\end{aligned}\right\} \tag{2.23}$$

$$\left.\begin{aligned} a_{3,0} &= -\sqrt{\tfrac{1}{10}}(2d_{15}+2d_{24}-2d_{33}+d_{31}+d_{32}),\\ a_{3,1} &= -\tfrac{1}{2\sqrt{30}}[(3d_{11}+d_{12}-4d_{13}+2d_{26}-8d_{35})\\ &\qquad - \mathrm{i}(3d_{22}+d_{21}-4d_{23}+2d_{16}-8d_{34})],\\ a_{3,2} &= \tfrac{1}{2\sqrt{3}}[(2d_{15}-2d_{24}-d_{32}+d_{31}) - 2\mathrm{i}(d_{36}+d_{14}+d_{25})]\\ \text{and}\quad a_{3,3} &= \tfrac{1}{2\sqrt{2}}[(d_{11}-d_{12}-2d_{26}) + \mathrm{i}(d_{22}-d_{21}-2d_{16})].\end{aligned}\right\} \tag{2.24}$$

3. Symmetry types of the linear piezoelectricity tensor

(a) Symmetries of deviators

The starting point for analyzing the symmetry of a physical tensor is the symmetry transformation. An orthogonal transformation is called a symmetry transformation of a tensor

if the tensor is invariant under this transformation. For the linear piezoelectricity tensor $\mathbf{d}$, the symmetry transformation $\mathbf{Q}$ means that

$$\mathbf{Q}^{\times 3}\mathbf{d} = \mathbf{d} \quad \text{or} \quad Q_{ip}Q_{jq}Q_{kr}d_{pqr} = d_{ijk}. \tag{3.1}$$

All the symmetry transformations of tensor $\mathbf{d}$ form a group, called the symmetry group of $\mathbf{d}$ and denoted by $G[\mathbf{d}]$.

Due to the property

$$\epsilon_{ijk}\epsilon_{pqr} = \begin{vmatrix} \delta_{ip} & \delta_{iq} & \delta_{ir} \\ \delta_{jp} & \delta_{jq} & \delta_{jr} \\ \delta_{kp} & \delta_{kq} & \delta_{kr} \end{vmatrix}, \tag{3.2}$$

the permutation tensor must (and at most) appear in an irreducible tensor and it further plays a role of making an even (odd)-order deviator into an odd (even)-order irreducible tensor, while every identity tensor δ_{ij} involved increases the tensor order by 2, i.e. equation (2.2). For more detailed discussions on this, one can refer to the paper by Zou *et al.* [9]. Thus, since the identity tensor is isotropic, the anisotropy of an irreducible tensor in a deviator $\mathbf{D}$ must be determined by $\mathbf{D}$ alone or its combination with a permutation tensor, expressed as $\boldsymbol{\epsilon}\mathbf{D}$ which may indicate

$$\boldsymbol{\epsilon} \otimes \mathbf{D} \text{ or } \boldsymbol{\epsilon} \cdot \mathbf{D}. \tag{3.3}$$

In summary, the symmetry group of a tensor can be derived from the intersection of the symmetry groups of all deviators, in the form $\mathbf{D}$ or $\boldsymbol{\epsilon}\mathbf{D}$, resulting in the irreducible decomposition of the tensor. For instance, we can express, from equation (2.2), the symmetry group of the linear piezoelectricity tensor $\mathbf{d}$ as

$$G[\mathbf{d}] = G[\mathbf{u}] \cap G[\mathbf{v}] \cap G[\boldsymbol{\epsilon}\mathbf{D}^{(2)}] \cap G[\mathbf{D}^{(3)}]. \tag{3.4}$$

Let $\mathbf{n}$ be a unit vector representing the normal to a plane and $\mathbf{m}$ be any vector perpendicular to $\mathbf{n}$, then $\mathbf{m} \cdot \mathbf{n} = 0$. Typically, one can choose two unit vectors $\mathbf{m}_1$ and $\mathbf{m}_2$ orthogonal to each other in such a plane to form, together with $\mathbf{n}$, a right-hand coordinate system $\{\mathbf{m}_1, \mathbf{m}_2, \mathbf{n}\}$. The vector $\mathbf{m}$ can be represented in general as

$$\mathbf{m}_\phi = \mathbf{m}_1 \cos\phi + \mathbf{m}_2 \sin\phi. \tag{3.5}$$

The reflection transformation in the plane normal to $\mathbf{n}$, denoted by $\mathbf{R}_\mathbf{n} = 1 - 2\mathbf{n} \otimes \mathbf{n}$, has the properties

$$\mathbf{R}_\mathbf{n}\mathbf{n} = -\mathbf{n}, \mathbf{R}_\mathbf{n}\mathbf{m}_\phi = \mathbf{m}_\phi, \quad \forall \phi \in [0, 2\pi). \tag{3.6}$$

It is easy to prove that a rotation $\mathbf{Q}(\theta, \mathbf{n})$ of angle θ about an axis $\mathbf{n}$ can be achieved by two reflection transformations. For example, for $\theta = 2\pi/k$, we have

$$\mathbf{Q}\left(\frac{2\pi}{k}\right)\mathbf{n} = \mathbf{R}_{\mathbf{m}_0}\mathbf{R}_{\mathbf{m}_{\pi/k}}. \tag{3.7}$$

As is well known, the deviator is the simplest tensor, and so we study the symmetry types of deviators of different orders first. A zeroth-order deviator (scalar) α is isotropic (K_h) and a first-order deviator (vector) $\mathbf{v}$ is transversely isotropic ($C_{\infty v}$ or T_2) while $\epsilon\alpha$ is hemitropic (K) and $\boldsymbol{\epsilon}\mathbf{v}$ is transversely hemitropic ($C_{\infty h}$ or T_3). For a single deviator of finite order, the symmetry type can be classified according to the symmetry or antisymmetry with respect to a given plane. A plane with normal $\mathbf{n}$ is referred to as the symmetry or antisymmetry mirror plane ($\mathrm{MP}^{+/-}$) of a pth-order deviator $\mathbf{D}^{(p)}$ if and only if the transformation relation takes the form

$$\mathbf{R}_\mathbf{n}^{\times p}\mathbf{D}^{(p)} = \mathbf{D}^{(p)} \quad \text{or} \quad \mathbf{R}_\mathbf{n}^{\times p}\mathbf{D}^{(p)} = -\mathbf{D}^{(p)}. \tag{3.8}$$

It is easy to prove that the identity tensor $\mathbf{1}$ and the permutation tensor ϵ satisfy

$$\mathbf{R}_\mathbf{n}^{\times 2}\mathbf{1} = \mathbf{1}, \quad \mathbf{R}_\mathbf{n}^{\times 3}\boldsymbol{\epsilon} = -\boldsymbol{\epsilon} \quad \forall \mathbf{n}, \tag{3.9}$$

and thus, they have ∞^3 MP^+s and ∞^3 MP^-s, respectively.

Table 1. Symmetry types of the second-order deviator $\boldsymbol{\epsilon} \cdot \mathbf{D}^{(2)}$.

MPs	symmetry groups	$\mathrm{MP}^{+/-}$s	axis direction set
overstepped	C_1, C_2		
orthogonal	D_2	3^-	$\{\mathbf{n}_3, \mathbf{n}_4\}$
tetragonal	C_S, C_{2v}, S_4, D_{2d}	3^-2^+	$\{\mathbf{n}, \mathbf{m} : \mathbf{n}\perp\mathbf{m}\}$
TI	$C_3, D_3, C_4, C_6, D_4, D_6, C_\infty, D_\infty$	$(\infty+1)^-$	$\{\mathbf{n}\}$
null	$C_{3v}, C_{3h}, D_{3h}, C_{4v}, C_{6v}, T, T_d, C_{\infty v}$	—	$A_3 = 0$

Because of the multipole representation (2.11), one can investigate the anisotropic structure of a deviator through its axis-direction set. A plane is said to be the MP^+ (MP^-) of an axis-direction set if the mirror of the axis-direction set with respect to the plane is invariant or becomes a set in which the even (odd) axis-directions change their signs when compared with their original ones. Thus as an MP^+, the axis-directions under the MP transformation are either unchanged, in other words, the axes must lie on the MP, or changed in pair(s). In the latter case, the pairs can both be perpendicular to the MP, or making the MP as their mid-separate surface. For the MP^-, besides the above cases, an additional axis-direction perpendicular to the MP is needed. Once the MPs of a deviator $\mathbf{D}$ are determined, the p MP^+s and q MP^-s of $\mathbf{D}$ will become p MP^-s and q MP^+s of $\boldsymbol{\epsilon}\mathbf{D}$ correspondingly (due to $(3.9)_2$).

Based on the above analysis, we can now derive three symmetry types for the second-order deviator $\boldsymbol{\epsilon} \cdot \mathbf{D}^{(2)}$ and seven symmetry types for the third-order deviator $\mathbf{D}^{(3)}$ as follows. A second-order deviator in the form $\boldsymbol{\epsilon} \cdot \mathbf{D}^{(2)}$ is at least orthogonal, tetragonal if $\mathbf{n}_3\perp\mathbf{n}_4$ and transversely isotropic (TI) if $\mathbf{n}_3||\mathbf{n}_4$. The corresponding symmetry groups of $\boldsymbol{\epsilon} \cdot \mathbf{D}^{(2)}$ (except for the non-piezoelectric groups), their MPs and axis-direction sets are listed in table 1. The results for a third-order deviator $\mathbf{D}^{(3)}$ are listed in table 2. As can be observed from table 2, there are seven types of symmetry:

I. Transverse isotropy (TI) if the three axis-directions are the same.
II. Tetragonal symmetry if the three axis-directions form a Cartesian coordinate frame.
III. Hexagonal symmetry if the three axis-directions are coplanar and have the same (120°) separation angle to each other.
IV. Orthogonal symmetry if one axis-direction is a principal direction of the other two.
V. Trigonal symmetry if the three axis-directions can be obtained by rotating an axis-direction around another one at 120°.
VI. Monoclinic symmetry if one axis-direction lies on a MP of the other two.
VII. Triclinic symmetry if no MP exists for the axis-direction set.

Also in table 2, the seven symmetry types of a single third-order deviator are numbered from I to VII, and their symmetry groups are called groups type I–VII which will be used as the framework for symmetry classification of the linear piezoelectricity tensor. From these discussions, we also find that the symmetry types of a single deviator can be distinguished simply through their numbers of $\mathrm{MP}^{+/-}$s.

(b) Symmetry types of a linear piezoelectricity tensor

A linear piezoelectricity tensor consists of at most two vectors, a second-order deviator and a third-order deviator without the isotropic part. From equation (3.4), we can obtain the symmetry types of the linear piezoelectricity tensor from the symmetry properties of the vectors, the second- and third-order deviators. The route to carry out the intersection can be described as follows:

— The intersection of two vectors results in two kinds of symmetries: the monoclinic (II) symmetry when the two vectors have distinct axis-directions, or the TI (VII) symmetry if the two vectors have the same axis-direction or one of them vanishes.

Table 2. Symmetry types of the third-order deviator $\mathbf{D}^{(3)}$. Note: for simplicity, the coplanar MP normals are hereinafter assumed to lie on the ($\mathbf{e}_1$, $\mathbf{e}_2$)-plane, and the single MP normal is set to be the $\mathbf{e}_3$ ($\mathbf{e}$)-axis.

classes/types	symmetry groups	$\mathrm{MP}^{+/-}$s	axis direction set
triclinic/I	C_1	null	$\{\mathbf{n}_5, \mathbf{n}_6, \mathbf{n}_7\}$
monoclinic/II	C_s	1^+	$\{\mathbf{n}(\pi/2, \varphi_1), \mathbf{n}(\theta_2, \varphi_2), \mathbf{n}(\theta_2, \varphi_2 + \pi)\}$
			or $\{\mathbf{n}(\pi/2, \varphi_1), \mathbf{n}(\pi/2, \varphi_2), \mathbf{n}(\pi/2, \phi_3)\}$
orthogonal/III	C_2, C_{2v}	2^+1^-	$\{\mathbf{e}, \mathbf{n}(\pi/2, \varphi_1), \mathbf{n}(\pi/2, \phi_2)\}$
			or $\{\mathbf{e}, \mathbf{n}(\theta, \varphi), \mathbf{n}(\theta, \varphi + \pi)\}$
trigonal/IV	C_3, C_{3v}	3^+	$\{\mathbf{n}(\theta, \phi + 2k\pi/3), k = 0, 1, 2\}$
hexagonal/V	D_3, C_{3h}, D_{3h}	4^+3^-	$\{\mathbf{n}(\pi/2, \varphi + k\pi/3), k = 0, 1, 2\}$
cubic/VI	D_2, S_4, D_{2d}, T, T_d	6^+3^-	$\{\mathbf{e}, \mathbf{n}(\pi/2, \varphi + k\pi/2), k = 0, 1\}$
TI/VII	$C_4, C_6, C_{4v}, C_{6v}, C_\infty, C_{\infty v}$	∞^+1^-	$\{\mathbf{e}\}$
null	D_4, D_6, D_∞	—	$A_4 = 0$

— The intersection of the two vectors and the third-order deviator does not yield any new symmetry type. Table 3 shows that the monoclinic symmetry of $\mathbf{u}$ and $\mathbf{v}$ may be combined with the monoclinic symmetry of $\mathbf{D}^{(3)}$ if their MP^+s are the same, and that the TI symmetry of $\mathbf{u}$ and $\mathbf{v}$ can be combined with the orthogonal, trigonal and TI symmetries of $\mathbf{D}^{(3)}$ without changing the symmetry type. However, combination of the TI symmetry of the two vectors with the hexagonal and cubic symmetries of $\mathbf{D}^{(3)}$ could reduce the symmetry to the trigonal and orthogonal symmetry, respectively.

— The intersection of $\mathbf{u}$, $\mathbf{v}$, $\mathbf{D}^{(3)}$ and $\boldsymbol{\epsilon} \cdot \mathbf{D}^{(2)}$ results in 15 irreducible symmetry types of linear piezoelectricity tensor, as shown in table 4 with the details being further discussed in the next subsection. The main points to construct the new type are the combination of the symmetry groups and the coupling of the axis-direction sets in tables 1 and 3. We should also point out that the remarkable property of the different symmetry types are their decisive number and pattern of $\mathrm{MP}^{+/-}$s, with the exception for trigonal type IV^-, tetragonal type VI^- and TI type VII^-. These three types are indistinguishable from the triclinic type I or monoclinic type III^- through their $\mathrm{MP}^{+/-}$s, as will be explained in detail in §4*b*.

With the detailed analysis on the symmetry types of the involved vectors and deviators, we are now in a position to answer the first key question. That is, why the number of the irreducible symmetry types in a linear piezoelectric tensor is larger than that in a linear elasticity tensor?

We note that the number of the symmetry types of a single third-order deviator cannot exceed that of a single fourth-order deviator. Even the intersection of two vectors and a third-order deviator does not yield a larger number of symmetry types than the intersection of two second-order deviators and a fourth-order deviator yields where the latter intersection completely determines the elasticity tensor. Thus, the complexity in the piezoelectricity tensor is due to the symmetry incompatibility between the second-order deviator and third-order deviator, which then results in a greater number of irreducible symmetry types in a linear piezoelectric tensor than that in the elasticity tensor.

Again, the 15 irreducible symmetry types for the linear piezoelectric tensor are listed in table 4, which contains important and useful information. For instance, from the patterns of the axis-direction sets in this table, one can count the numbers of modular and angular variables for every symmetry type. We point out that attention should be paid that in a natural coordinate system, there are two or three pre-determined angular variables. For example, the tetragonal type VI^+ with symmetry group $\{T, T_d\}$ is usually treated as having only one independent variable. Thus

Table 3. Intersection of **u**, **v** and $\mathbf{D}^{(3)}$. Note: the module within a square bracket means that the corresponding deviator is optional.

classes/types	symmetry groups	$MP^{+/-}s$	axis direction sets
triclinic/I	C_1	null	$[A_1]\{\mathbf{n}_1\}[A_2]\{\mathbf{n}_2\}A_4\{\mathbf{n}_5, \mathbf{n}_6, \mathbf{n}_7\}$
monoclinic/II	C_s	1^+	$[A_1]\{\mathbf{n}(\pi/2, \varphi_4)\}[A_2]\{\mathbf{n}(\pi/2, \varphi_5)\}$ A_4 $\{\mathbf{n}(\pi/2, \varphi_1), \mathbf{n}(\theta_2, \varphi_2), \mathbf{n}(\theta_2, \varphi_2 + \pi)\}$ or $\{\mathbf{n}(\pi/2, \varphi_1), \mathbf{n}(\pi/2, \varphi_2), \mathbf{n}(\pi/2, \varphi_3)\}$
orthogonal/III	C_2, C_{2v}	2^+1^-	$[A_1]\{\mathbf{e}\}[A_2]\{\mathbf{e}\}$ A_4 $\{\mathbf{e}, \mathbf{n}(\theta, \varphi), \mathbf{n}(\theta, \varphi + \pi)\}$ or $\{\mathbf{e}, \mathbf{n}(\pi/2, \phi_1), \mathbf{n}(\pi/2, \varphi_2)\}$
trigonal/IV	C_3, C_{3v}	3^+	$[A_1]\{\mathbf{e}\}[A_2]\{\mathbf{e}\}$ $A_4\{\mathbf{n}(\theta, \varphi + 2\pi/3), k = 0, 1, 2\}$
hexagonal/V	D_3, C_{3h}, D_{3h}	4^+3^-	$A_4\{\mathbf{n}(\pi/2, \varphi + k\pi/3), k = 0, 1, 2\}$
cubic/VI	D_2, S_4, D_{2d}, T, T_d	6^+3^-	$A_4\{\mathbf{e}, \mathbf{n}(\pi/2, \varphi + k\pi/2), k = 0, 1\}$
TI/VII	$C_4, C_6, C_{4v}, C_{6v}, C_{\infty v}, D_{\infty}, C_{\infty}\backslash cr$	∞^+1^-	$[A_1]\{\mathbf{e}\}[A_2]\{\mathbf{e}\}[A_4]\{\mathbf{e}\}$
null	D_4, D_6, D_{∞}	–	$A_1 = A_2 = A_4 = 0$

when getting back to the omitted angular variables, the modular variable and angular one (in the parentheses) are counted separately, as listed in table 5, for the whole independent variables of different symmetry types.

(c) Characteristic web tree of the linear piezoelectricity tensor

It is well known that a symmetry group may contain some other symmetry groups inside so that it possesses a relatively higher symmetry. Among the 23 piezoelectric symmetry groups, the triclinic group which only possesses the identity transformation has the lowest symmetry. With the insertion of an additional transformation, the number of independent variables in the linear piezoelectricity tensor may be reduced, and the corresponding axis-direction sets are specialized. In so doing, all possible consequences finally generate a characteristic web tree.

In order to draw the characteristic web tree, some definitions are presented first. For two basic symmetry groups A and B, if $A \subset B$, then A is called the *subgroup* of B, and B the *mother group* of A. B is called the *nearest* mother group of A if there is no other mother group of A contained by B. A symmetry group B is called the *eigengroup* of a symmetry type of a tensor **T** if no mother group results in the same symmetry type of the tensor **T**. A symmetry group is called the *null group* of a tensor if there is no symmetry type of the tensor which is invariant under all transformations of the symmetry group, except for the special case where all components of the tensor vanish. A symmetry group is said to be an *overstepped group* of a tensor if the most generic symmetry type of the tensor possesses a higher symmetry group than it.

According to these definitions, some basic propositions can be described: except for the null case, every symmetry type of a tensor has only one eigengroup. If a symmetry group is a null group of a tensor, all its mother groups, and all its subgroups that are not overstepped or belong to any symmetry type are also null groups of the tensor. If a symmetry group is an overstepped group, all its subgroups are also overstepped groups of the tensor. For examples, among the piezoelectric symmetry groups, for a vector, $C_{\infty v}$ is overstepped and D_2, D_3, C_{3h} and S_4 are null; for a second-order deviator, C_2 is overstepped and C_{3v}, C_{3h}, C_{4v} and T are null; for a third-order deviator, D_4 and D_6 are null.

Table 4. Symmetry types of a linear piezoelectricity tensor.

classes/types	symmetry groups	$MP^{+/-}$s	pattern of axis direction sets
triclinic/I	C_1	null	$[A_1]\{\mathbf{n}_1\}[A_2]\{\mathbf{n}_2\}$ $[A_3]\{\mathbf{n}_3, \mathbf{n}_4\}$ $A_4\{\mathbf{n}_5, \mathbf{n}_6, \mathbf{n}_7\}$
monoclinic/II	C_s	1^+	$[A_1]\mathbf{n}(\pi/2, \varphi_1)[A_2]\mathbf{n}(\pi/2, \varphi_2)$ $[A_3]\{\mathbf{e}, \mathbf{n}(\pi/2, \varphi_3)\}$ A_4 $\{\mathbf{n}(\pi/2, \varphi_1), \mathbf{n}(\pi/2, \varphi_2), \mathbf{n}(\pi/2, \varphi_3)\}$ or $\{\mathbf{n}(\pi/2, \varphi_4), \mathbf{n}(\theta, \varphi_5 + k\pi), k = 0, 1\}$
monoclinic/III$^-$	C_2	1^-	$[A_1]\{\mathbf{e}\}[A_2]\{\mathbf{e}\}$ A_3 $\{\mathbf{n}(\pi/2, \varphi_1), \mathbf{n}(\pi/2, \varphi_2)\}$ or $\{\mathbf{n}(\theta_1, \varphi_1 + k\pi), k = 0, 1\}$ A_4 $\{\mathbf{e}, \mathbf{n}(\pi/2, \varphi_3), \mathbf{n}(\pi/2, \varphi_4)\}$ or $\{\mathbf{e}, \mathbf{n}(\theta_2, \varphi_3 + k\pi), k = 0, 1\}$
orthogonal/III	C_{2v}	2^+1^-	$[A_1]\{\mathbf{e}\}[A_2]\{\mathbf{e}\}$ $[A_3]\{\mathbf{n}(\pi/2, \varphi_1 + k\pi/2), k = 0, 1\}$ $\{\mathbf{e}, \mathbf{n}(\pi/2, \varphi_2), \mathbf{n}(\pi/2, \varphi_3)\}$ A_4 or $\{\mathbf{e}, \mathbf{n}(\theta, \varphi_2 + k\pi), k = 0, 1\}$ or $\{\mathbf{e}, \mathbf{n}(\pi/3, \varphi + k\pi), k = 0, 1\}$
orthogonal/III$^+$	D_2	3^- perpendicular	$A_3\{\mathbf{n}(\theta, \varphi + k\pi), k = 0, 1\}$ $A_4\{\mathbf{e}, \mathbf{n}(\pi/2, \varphi + k\pi/2), k = 0, 1\}$
trigonal/IV$^-$	C_3	null	$[A_1]\{\mathbf{e}\}[A_2]\{\mathbf{e}\}$ $A_3\{\mathbf{e}\}$ $A_4\{\mathbf{n}(\theta, \varphi + 2k\pi/3), k = 0, 1, 2\}$
trigonal/IV	C_{3v}	3^+	$[A_1]\{\mathbf{e}\}[A_2]\{\mathbf{e}\}$ $A_4\{\mathbf{n}(\theta, \varphi + 2k\pi/3), k = 0, 1, 2\}$
trigonal/V$^-$	D_3	3^- coplanar	$A_3\{\mathbf{e}\}$ $A_4\{\mathbf{n}(\pi/2, \varphi + k\pi/3), k = 0, 1, 2\}$
hexagonal/V	C_{3h}, D_{3h}	4^+3^-	$A_4\{\mathbf{n}(\pi/2, \varphi + k\pi/3), k = 0, 1, 2\}$
tetragonal/VI$^-$	S_4	1^-	$A_3\{\mathbf{n}(\pi/2, \varphi_1 + ((2k+1)\pi/4)), k = 0, 1\}$ $A_4\{\mathbf{e}, \mathbf{n}(\pi/2, \varphi_2 + k\pi/2), k = 0, 1\}$
tetragonal/VI	D_{2d}	2^+3^-	$A_3\{\mathbf{n}(\pi/2, \varphi + ((2k+1)\pi/4)), k = 0, 1\}$ $A_4\{\mathbf{e}, \mathbf{n}(\pi/2, \varphi + k\pi/2), k = 0, 1\}$
cubic/VI$^+$	T, T_d	6^+3^-	$A_4\{\mathbf{e}, \mathbf{n}(\pi/2, \varphi + k\pi/2), k = 0, 1\}$
TI/VII$^-$	C_4, C_6, C_∞	1^-	$[A_1]\{\mathbf{e}\}[A_2]\{\mathbf{e}\}A_3\{\mathbf{e}\}A_4\{\mathbf{e}\}$
TI/VII	$C_{4v}, C_{6v}, C_{\infty v}$	∞^+1^-	$[A_1]\{\mathbf{e}\}[A_2]\{\mathbf{e}\}A_4\{\mathbf{e}\}$
TI/VII$^+$	D_4, D_6, D_∞	$(\infty + 1)^-$	$A_3\{\mathbf{e}\}$

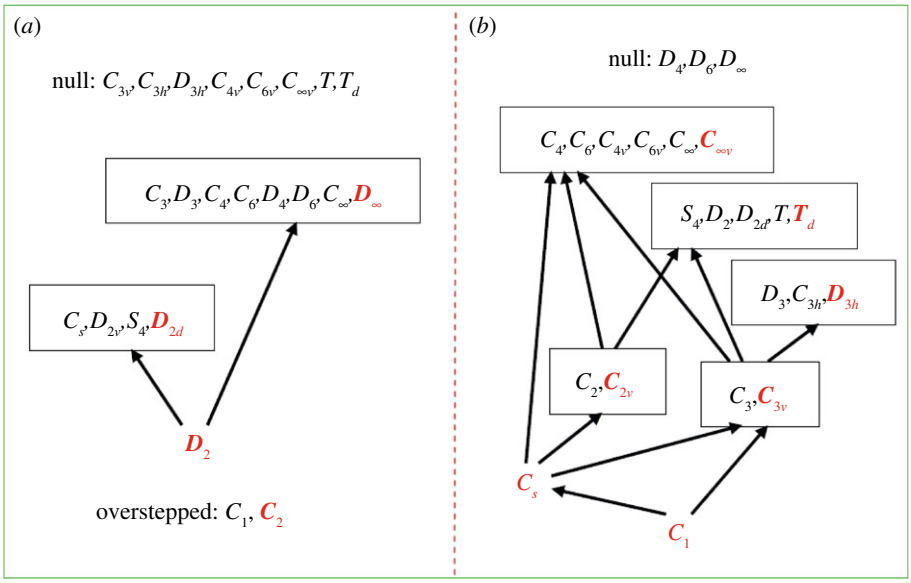

Figure 1. Characteristic web trees of a second-order deviator $\epsilon \cdot \mathrm{D}^{(2)}$ (*a*) and a third-order deviator $\mathrm{D}^{(3)}$ (*b*), where the symmetry groups marked in bold with a large font in red are the eigengroups of the corresponding symmetry types and all non-piezoelectric symmetry groups are omitted. (Online version in colour.)

Table 5. Independent modular and angular variables of a linear piezoelectricity tensor.

classes/types	TI/VII$^+$	TI/VII	TI/VII$^-$	cubic/VI$^+$	tetragonal/VI
numbers	1(2)	1–3(2)	2–4(2)	1(3)	2(3)
classes/types	tetragonal/VI$^-$	hexagonal/V	trigonal/V$^-$	trigonal/IV	trigonal/IV$^-$
numbers	2(4)	1(3)	2(3)	1–3(4)	2–4(4)
classes/types	orthogonal/III$^+$	orthogonal/III	monoclinic/III$^-$	monoclinic/II	triclinic/I
numbers	2(4)	1–4(4)	2–4(6)	1–4(5–8)	1–4(6–14)

We first elaborate the characteristic web trees (figure 1) of a single deviator. For a second-order deviator $\mathbf{D}^{(2)}$ in the appearance of $\boldsymbol{\epsilon} \cdot \mathbf{D}^{(2)}$, let us begin with the lowest orthogonal symmetry group D_2 : (i) consider three nearest mother groups D_4, D_6 and D_{2d} in the up routine of the web tree, we find that D_{2d} results in $\mathbf{n}_3 \perp \mathbf{n}_4$ while both D_4 and D_6 make $\mathbf{n}_3 = \mathbf{n}_4$ so that two higher symmetry types over the generic one happen; (ii) list the subgroups of D_4, D_6 and D_{2d} other than D_2, and check whether they are overstepped or belong to the lower symmetry types. If not, say C_4 of D_4, C_3, D_3 and C_6 of D_6, and C_s, C_{2v} and S_4 of D_{2d}, we can confirm that they must result in the same symmetry types as their mother groups and add them to the corresponding symmetry types; (iii) investigate the next nearest mother groups of D_4, D_6 and D_{2d}. Here, we have only D_∞ of both D_4 and D_6 since T_d of D_{2d} is null. We see no new symmetry type associated with D_∞, so we add it and its subgroup C_∞ to the same type; (iv) continue until the null or eigengroup is reached. If some new symmetry types appear, we then repeat from step (ii); (v) find out the symmetry groups of every type whose mother groups do not appear entirely, say C_3 and C_4, and mark all the omitted mother groups of them to be null; (vi) modify the characteristic web tree according to the eigengroups after finding the positions for all the possible symmetry groups. Namely a symmetry type α is said to be higher than β if the eigengroup of α contains that of β. Finally, we obtain the characteristic web tree of $\boldsymbol{\epsilon} \cdot \mathbf{D}^{(2)}$ with three symmetry types as shown in figure 1*a*. We remark that in judging the new symmetry types, the visual pattern of the axis-direction set is very

helpful. For the third-order deviator $\mathbf{D}^{(3)}$, we begin with the lowest triclinic symmetry of group C_1, follow the same steps as above, and then derive its seven symmetry types and construct its characteristic web tree as shown in figure 1*b*.

For a single vector there is only TI type with the eigengroup $C_{\infty v}$. The groups type I, II, III, IV and all the groups in type VII but $C_{\infty v}$ are overstepped, while groups type V and VI become null. In combining the two vectors, the group C_s will separate itself out to be monoclinic type, and most groups are in the overstepped state except for groups type I, II which are stepped up to the TI type. Thus, since we know that the groups of symmetry types of a single third-order deviator is totally the subset of those of two vectors, further combination of two vectors with a third-order deviator does not produce any new symmetry type other than those of a single third-order deviator. For instance, the group types I, V and VI revive from the overstepped and null states, respectively, when the third-order deviator appears, type II of the third-order deviator can coexist with the monoclinic type of two vectors, and the TI type of two vectors may participate into the types III, IV and VII of a third-order deviator.

Finally, the combination of two vectors, a second-order deviator and a third-order deviator is complicated. Two fundamental features should be noticed: (i) the detached groups must be detached after the combination; (ii) the routes of eigengroups in the web trees must be unchanged, and the groups with a higher position in the original web tree cannot have a lower position in the new web tree. Thus, using the notations given in table 4, groups C_2, C_3, D_3 and S_4 have to be separated out to form types III$^-$, IV$^-$, V$^-$ and VI$^-$ individually, and the original eigengroups D_2, D_{2d}, C_1, C_s, C_{2v} and C_{3v} will still stay in the types III$^+$,VI, I, II, III and IV. For types with several groups, the results are: type V with C_{2h} and D_{3h}, and type VI$^+$ with T and T_d are given by a single third-order deviator while type VII$^+$ with D_4, D_6 and D_∞ is given by a single second-order deviator; type VII with C_{4v}, C_{6v} and $C_{\infty v}$ is defined by two vectors and a third-order deviator, and in type VII with C_4, C_6 and C_∞, both the second- and third-order deviators exist. *Therefore, as the answer to the second key question, we have finally obtained 15 irreducible symmetry types* in seven classes for two vectors $\mathbf{u}$ and $\mathbf{v}$, a second-order deviator $\mathbf{D}^{(2)}$ in the form $\boldsymbol{\epsilon}\cdot\mathbf{D}^{(2)}$ and a third-order deviator $\mathbf{D}^{(3)}$. When the evolving routes between different symmetry types are determined, the characteristic web tree of the linear piezoelectricity tensor can be illustrated in figure 2.

4. Symmetry identification of the linear piezoelectricity tensor

(a) Two kinds of modulus

From the Frobenius norm

$$\left\|\mathbf{D}^{(p)}\right\| = \sqrt{D_{i_i\cdots i_p}D_{i_i\cdots i_p}} = \sqrt{a_{p,0}^2 + 2\sum_{k=1}^{p} a_{p,r}\bar{a}_{p,r}} = |A|\,\left\|\lfloor \mathbf{n}_1\otimes\cdots\otimes\mathbf{n}_p\rfloor\right\| \tag{4.1}$$

for a pth-order deviator, we know that the norm is actually the product of two kinds of modulus, namely, the scalar module A and the phase module B defined as

$$B = \left\|\lfloor \mathbf{n}_1\otimes\cdots\otimes\mathbf{n}_p\rfloor\right\|. \tag{4.2}$$

While the scalar module determines the existence of the deviator, the phase module contains certain information on its axis-direction set. For example, the phase part of a second-order deviator with axis-direction set $\{\mathbf{n}_3,\mathbf{n}_4\}$ takes the form

$$\lfloor \mathbf{n}_3\otimes\mathbf{n}_4\rfloor = \tfrac{1}{2}(\mathbf{n}_3\otimes\mathbf{n}_4+\mathbf{n}_4\otimes\mathbf{n}_3) - \tfrac{1}{3}\gamma_{34}\mathbf{1}, \tag{4.3}$$

where $\gamma_{34}=\mathbf{n}_3\cdot\mathbf{n}_4$. The corresponding phase module has the span

$$B = \sqrt{\tfrac{1}{2}+\tfrac{1}{6}\gamma_{34}^2} \in [\tfrac{1}{\sqrt{2}},\sqrt{\tfrac{2}{3}}] \approx [0.7071, 0.8165], \tag{4.4}$$

where the maximum corresponds to the TI symmetry, the minimum to the tetragonal symmetry and any value in between means the orthogonal symmetry.

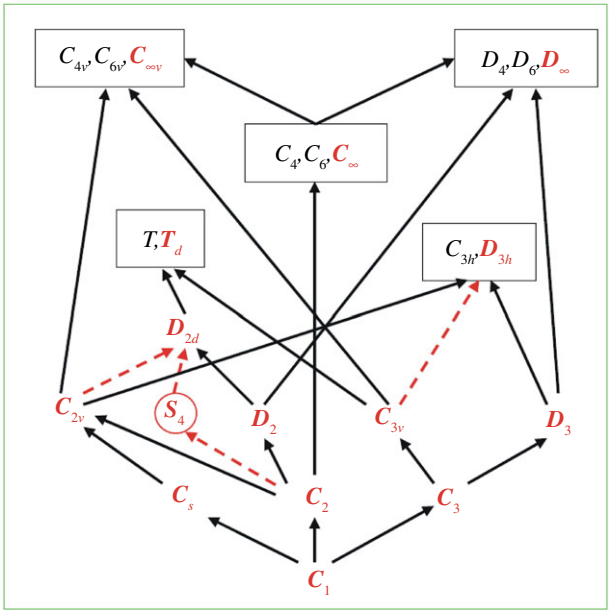

Figure 2. Characteristic web tree of the linear piezoelectricity tensor, where the symmetry groups marked in bold with a large font size are the 15 eigen or irreducible groups of the corresponding symmetry types, and the symmetry group within the circle and route arrows in dashed lines are the modification to the result given by Geymonat & Weller [7]. (Online version in colour.)

A third-order deviator with axis-direction set $\{\mathbf{n}_5, \mathbf{n}_6, \mathbf{n}_7\}$ has its phase-part expression as

$$\lfloor \mathbf{n}_5 \otimes \mathbf{n}_6 \otimes \mathbf{n}_7 \rfloor = \tfrac{1}{6}\langle \mathbf{n}_5 \otimes \mathbf{n}_6 \otimes \mathbf{n}_7 \rangle - \tfrac{1}{15}[\gamma_{56}\langle 1 \otimes \mathbf{n}_7 \rangle + \gamma_{57}\langle 1 \otimes \mathbf{n}_6 \rangle + \gamma_{67}\langle 1 \otimes \mathbf{n}_5 \rangle], \tag{4.5}$$

where the symbol '$\langle\cdot\rangle$' is again the symmetrization operator without dividing by the number of the involved terms. The phase module of equation (4.5) depends on three cosines γ_{ij} $(5 \le i \ne j \le 7)$ and its generic formula is complicated. For the third-order deviators with TI or tetragonal symmetries, their phase parts simply become

$$\mathbf{n}^{\otimes 3} - \tfrac{1}{5}\langle \mathbf{1} \otimes \mathbf{n} \rangle \quad \text{or} \quad \tfrac{1}{6}\langle \mathbf{n} \otimes \mathbf{m}_1 \otimes \mathbf{m}_2 \rangle. \tag{4.6}$$

Thus, the phase module has the maximum $\sqrt{\frac{2}{5}} \approx 0.6325$ and minimum $\sqrt{\frac{1}{6}} \approx 0.4082$. It is interesting to point out that they actually represent two kinds of the highest symmetries.

(b) Identification of the linear piezoelectric tensor using indicators

In this subsection, we will develop the identification method for the linear piezoelectric tensor as the answer to our third and finally key question in this paper. It is based on the following facts: (1) the anisotropy of a deviator is determined by its phase part; (2) since the symmetry type of a deviator can be distinguished by its $\mathrm{MP}^{+/-}$s, most symmetry types of the linear piezoelectricity tensor can then be identified by its $\mathrm{MP}^{+/-}$s; others need further investigation on the deviators in their irreducible decomposition; (3) the **e**-axis is the normal of the $\mathrm{MP}^{+/-}$ ($\mathrm{MP}^{-/+}$) of an odd (even)-order deviator if and only if its components in the orthonormal bases (2.16) satisfy the condition $a_{p,2k/2k+1} = 0$, $k = 0, 1, \ldots, [p/2]$. Therefore, one can make use of the zero points of the sum of the component modulus normalized by the Frobenius norm to identify the $\mathrm{MP}^{+/-}$s of a deviator, and also can extend this approach to the linear piezoelectricity tensor as a set of deviators. This is explained in detail below.

It is noted that the components $a_{p,r}(r=-p,\ldots,p)$ in equation (2.17) of a deviator $\mathbf{D}^{(p)}$ are functions of two Euler angles θ and φ when the rotation transformation

$$\mathbf{R}(0,\theta,\varphi)=\mathbf{Q}(\theta,\mathbf{e}_2)\mathbf{Q}(\varphi,\mathbf{e}), \tag{4.7}$$

is applied on the frame $\{\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}\}$; but

$$a_{p,0}^2+2\sum_{k=1}^{[p/2]}(|a_{p,2k}|^2+|a_{p,2k+1}|^2)=\|\mathbf{D}^{(p)}\|^2$$

is invariant. Thus, the judgment on MP$^{+/-}$s of the deviator must be mutually complementary. That is, by introducing the normalized indicators

$$C_D(\theta,\varphi)=\|\mathbf{D}^{(p)}\|^{-2}\left[a_{p,0}^2+2\sum_{k=1}^{[p/2]}|a_{p,2k}|^2\right]\quad\text{or}\quad 2\|\mathbf{D}^{(p)}\|^{-2}\sum_{k=1}^{[p/2]}|a_{p,2k+1}|^2, \tag{4.8}$$

we conclude that if $C_D(\theta,\varphi)=0$ for the MP$^+$s, then $C_D(\theta,\varphi)=1$ for the MP$^-$s, and vice versa. Thus, using the components calculated from equations (2.21) to (2.24) for the linear piezoelectricity tensor $\mathbf{d}$, equation (4.8) becomes

$$NC(\theta,\varphi)=\frac{2}{\|\mathbf{u}\|^2}|a_{1,1}^{\mathrm{u}}|^2+\frac{2}{\|\mathbf{v}\|^2}|a_{1,1}^{\mathrm{v}}|^2+\frac{2}{\|\mathbf{D}^{(2)}\|^2}|a_{2,1}|^2+\frac{2}{\|\mathbf{D}^{(3)}\|^2}(|a_{3,1}|^2+|a_{3,3}|^2), \tag{4.9}$$

where N is the number of the nonzero scalar modulus. In equation (4.9), the indicator $C(\theta,\varphi)$ will be zero for an MP$^-$ and maximum 1 for an MP$^+$. If the MP$^{+/-}$ is null or there is only one MP$^-$, two auxiliary indicators

$$\left.\begin{aligned} N_{\mathrm{odd}}C_{\mathrm{odd}}(\theta,\varphi)&=\frac{2}{\|\mathbf{u}\|^2}|a_{1,1}^{\mathbf{u}}|^2+\frac{2}{\|\mathbf{v}\|^2}|a_{1,1}^{\mathrm{v}}|^2+\frac{2}{\|\mathbf{D}^{(3)}\|^2}(|a_{3,1}|^2+|a_{3,3}|^2)\\ \text{and}\qquad C_{\mathrm{even}}(\theta,\varphi)&=\frac{2}{\|\mathbf{D}^{(2)}\|^2}|a_{2,1}|^2,\end{aligned}\right\} \tag{4.10}$$

are needed. In equations (4.9) and (4.10), a deviator term will disappear if its scalar module is zero. It is obvious that all the indicators in equations (4.9) and (4.10) are nonnegative and are further independent of the four scalar modules A_1 to A_4.

According to table 4, most symmetry types can be identified by $C(\theta,\varphi)$ (figure 3). If the MP$^{+/-}$ of $C(\theta,\varphi)$ is null (figure 3*a*,*m*) but $C_{\mathrm{odd}}(\theta,\varphi)$ has three coplanar MP$^+$s and $C_{\mathrm{even}}(\theta,\varphi)$ is TI on the same plane (figures 4*a* and 5*a*), then the symmetry type is trigonal type IV$^-$; otherwise, it is triclinic. If $C(\theta,\varphi)$ has only one MP$^-$ (figure 3*a*,*i*,*o*), then the symmetry type is: (i) tetragonal type VI$^-$ if both $C_{\mathrm{odd}}(\theta,\varphi)$ and $C_{\mathrm{even}}(\theta,\varphi)$ are tetragonal (namely have two MP$^+$ and two MP$^-$ normals) on the plane (figures 4*b* and 5*b*); (ii) TI type VII$^-$ if both $C_{\mathrm{odd}}(\theta,\varphi)$ and $C_{\mathrm{even}}(\theta,\varphi)$ are TI on the plane (figures 4*c* and 5*c*); (iii) otherwise, it is monoclinic type III$^-$.

It is easy to confirm that the indicators have the symmetry of centre inversion, so the entire information on them can be shown in the upper hemisphere. Thus, through the mapping

$$x=\mathrm{e}^{\mathrm{i}\varphi}\tan\frac{\theta}{2}, \tag{4.11}$$

we can plot the indicators on a unit disk. Some typical results on the modular parameters are listed in table 6 (the phase modules of vectors always equal to unit) and the images of the indicators are shown in figure 3. The piezoelectricity coefficients in their natural material coordinate system are taken from Newnham [1], Chen *et al.* [14] and the IEEE Standard on Piezoelectricity (1988) [15], listed in appendix A for easy future reference, including four fictive materials. In figure 3, we show also the images of the four fictive materials to make up the missing symmetry types. These are the type II by setting d_{31}, d_{32}, d_{33}, d_{14}, d_{15}, d_{24}, d_{25} and d_{36} to be zero in the right-hand quartz (YXwl), type IV$^-$ by adding $d_{11}=6$ and $d_{25}=16$, type V by letting d_{31}, d_{33} and d_{15} equal to zero (all based on material $LiTaO_3$), and type VI$^-$ by setting $d_{31}=7$ and $d_{15}=-0.8$ in material KH_2PO_4.

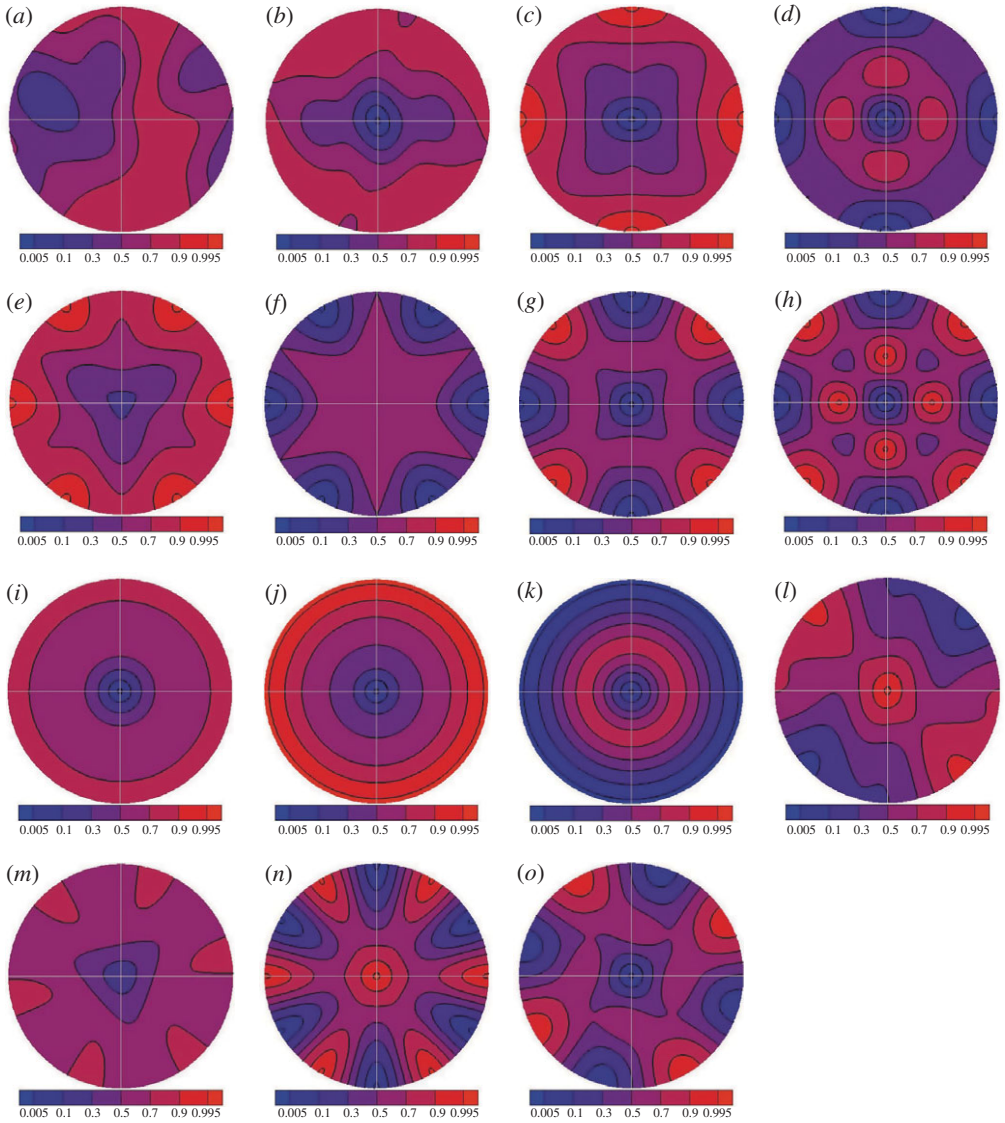

Figure 3. $C(\theta, \varphi)$ of various piezoelectric materials, where the last four materials *l*–*o* are fictive. Ten symmetry types can be identified directly from the number and pattern of their $MP^{+/-}$s, except for the trigonal type IV^-, tetragonal type VI^- and TI type VII^-. For these three symmetry types, we need the auxiliary indicators $C_{odd}(\theta, \phi)$ and $C_{even}(\theta, \phi)$, as shown in figures 4 and 5, to distinguish them from two lower symmetry types, triclinic type I and monoclinic type III^-, respectively. (*a*) Right-hand quartz (Yxw|) type I, (*b*) sucrose type III^-, (*c*) $PbNb_2O_6$ type III, (*d*) wood type III^+, (*e*) $LiTaO_3$ type IV, (*f*) α-quartz type V^-, (*g*) KH_2PO_4 type VI, (*h*) GaAs type VI^+, (*i*) $LiIO_2$ type VII^-, (*j*) ZnO type VII, (*k*) TeO_2 type VII^+, (*l*) fictive type II, (*m*) fictive type IV^-, (*n*) fictive type V and (*o*) fictive type VI^-. (Online version in colour.)

Since the properties of the number and pattern of $MP^{+/-}$s are invariant under transformation of the coordinate system, we can actually use the indicators for the identification of the linear piezoelectricity tensor measured in its natural coordinate system or in an arbitrarily oriented coordinate system.

We point out that there is actually another approach similar to that proposed for the linear elasticity tensor [11], which can be used to identify the piezoelectric tensor. That is, one can construct an explicit and analytical procedure from the solved axis-direction sets of the four deviators of the linear piezoelectricity tensor to judge $MP^{+/-}$s, identify the symmetry type and

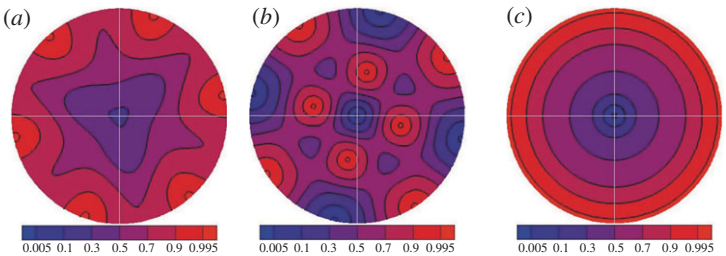

Figure 4. $C_{\mathrm{odd}}(\theta, \varphi)$ of materials *m*, *o* and *i* in figure 3. (*a*) Fictive type IV$^-$, (*b*) fictive type VI$^-$ and (*c*) $LiIO_2$ type VII$^-$. (Online version in colour.)

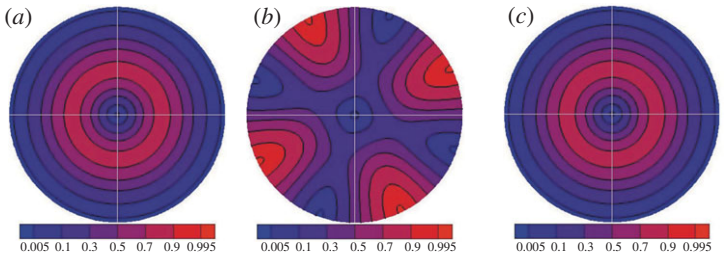

Figure 5. $C_{\mathrm{even}}(\theta, \varphi)$ of materials *m*, *o* and *i* in figure 3. (*a*) Fictive type IV$^-$, (*b*) fictive type VI$^-$ and (*c*) $LiIO_2$ type VII$^-$. (Online version in colour.)

Table 6. Modules of linear piezoelectricity materials (unit of scalar modulus: 10^{-12}C/N).

materials		$\{\mathbf{u}, \mathbf{v}\}$		$\mathbf{D}^{(2)}$		$\mathbf{D}^{(3)}$	
names	classes/types	A_1	A_2	A_3	B_3	A_4	B_4
right-hand quartz (YXwl) C_1	triclinic/I	0.2829×10^{-3}	0.4243×10^{-3}	0.3628	0.8161	9.231	0.5
sucrose C_2	monoclinic/III$^-$	0.868	1.902	0.5708	0.7669	2.663	0.4992
$PbNb_2O_6$ C_{2v}	orthogonal/III	30.6	66.4	24	0.7071	134	0.5274
wood D_2	orthogonal/III$^+$	0	0	0.1217	0.8055	0.19	0.4082
$LiTaO_3$ C_{3v}	trigonal/IV	5.8	10.2	0	—	45.93	0.4368
α-quartz D_3	trigonal/V$^-$	0	0	0.335	0.8165	9.2	0.5
KH_2PO_4 D_{2d}	tetragonal/VI	0	0	6.567	0.7071	23.6	0.4082
GaAs T_d	tetragonal/VI$^+$	0	0	0	—	7.8	0.4082
$LiIO_2$ C_6	TI/VII$^-$	14.52	31.87	3.65	0.8165	36.1	0.6325
ZnO C_{4v}	TI/VII	0.14	0.99	0	—	25.7	0.6325
TeO_2 D_4	TI/VII$^+$	0	0	4.05	0.8165	0	—

recover the rotation transformation $\mathbf{R}(\phi, \theta, \varphi)$ with three Euler angles ϕ, θ and φ to trace back to the tensor's natural coordinate system. This is simply confirmed by observing the axis-direction sets from tables 1 and 2 to tables 3 and 4, and can be realized with a short Fortran code so the MP$^{+/-}$s are identified. Then, from the final MP$^{+/-}$s, except for the trivial triclinic case, the transformation $\mathbf{R}(\phi, \theta, \varphi)$ back to the original natural coordinate system can be achieved as follows:

— Selecting a direction $\mathbf{n}(\theta, \phi)$ defined by two Euler angles θ, φ: For the types with only one MP$^+$ or MP$^-$, say types II, III$^-$ and VII$^-$, $\mathbf{n}$ is simply the normal of the MP$^+$ or MP$^-$

plane; for the types with more than two $MP^{+/-}$ normals on a plane, say types IV, V^-, V, VI, VI^+, VII and VII^+, it is the normal to the plane to be selected (especially for type IV^-, the $MP^{+/-}$ normals of the second- and third-order deviators should be considered); for types III and III^+ with three $MP^{+/-}$ normals perpendicular to each other, any one of them can be selected.

— Determining the third Euler angle, or equivalently the direction $\mathbf{m}_1$ on the plane normal to $\mathbf{n}$. For types II, III, IV^-, VI^-, VII^-, VII and VII^+, the third Euler angle is arbitrary and can be set to be zero; for types III, III^+, IV, V^- and V, $\mathbf{m}_1$ can be any coplanar $MP^{+/-}$ normal; for types VI and VI^+, $\mathbf{m}_1$ is usually chosen as one of $\mathbf{D}^{(3)}$'s axis-directions on the plane.

5. Concluding remarks

In this paper, the number of irreducible symmetry types of the linear piezoelectricity tensor has been proved to be 15. Furthermore, two methods have been proposed to identify the symmetry type of a linear piezoelectricity tensor measured in an arbitrarily oriented coordinate system. Through decomposing the linear piezoelectricity tensor into the irreducible parts formed by at most two vectors, a second- and a third-order deviators, and expressing each deviator by a scalar and an axis-direction set, the symmetry groups of a linear piezoelectric tensor can be obtained as the intersection of the symmetry groups of its deviators. By virtue of the mirror symmetry and antisymmetry ($MP^{+/-}$), the symmetry types of all deviators can be distinguished exactly, and the combination analyses result in 15 symmetry types of the linear piezoelectricity tensor. By expressing the components of a deviator in terms of the orthonormal base, the $MP^{+/-}$s of the deviator can be defined as the minimal/maximal points of a normalized characteristic function with respect to two Euler angles, and so its symmetry type can be identified. We have introduced an indicator so that the symmetry type of a linear piezoelectricity tensor can be determined by the indicator in the most common cases, and by two auxiliary indicators in some special cases. We have also proposed another method for identifying the symmetry type of a linear piezoelectricity tensor. It is based on the precise analyses of the solved axis-direction sets, and in this procedure, the rotation transformation back to the natural coordinate system is also available.

We point out that the developed methods will be particularly useful for symmetry identification of an unknown piezoelectric material and for possible back calculation of the involved piezoelectric coefficients. Furthermore, the methodology developed in this article for classifying the symmetry is universal and can be extended to any higher-order matter tensor.

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Appendix A. Piezoelectric material properties used in this paper

In most literature, the piezoelectric coefficients were defined as

$$d_{iI} = \begin{cases} d_{ijk}, j = k; & I = 1, 2, 3 \\ 2d_{ijk}, j \neq k; & I = 4, 5, 6. \end{cases} \tag{A 1}$$

This is convenient for matrix operation, but inconvenient for tensor operation. Thus, in this paper, we will not follow the definition by equation (A 1). In other words, in this paper, the coefficients d_{iI}, $I = 4, 5, 6$ will not be doubled as in equation (A 1), but will just be their original values (i.e. $d_{iI} = d_{ijk}$, $j \neq k$; $I = 4, 5, 6$). The unit of all the piezoelectricity coefficients is in 10^{-12}C/N.

The piezoelectric material with generic anisotropy material is the right-hand quartz (YXwl)

$$(d_{iI}) = \begin{pmatrix} 0.895 & -0.281 & -0.614 & -0.551 & -1.186 & -1.766 \\ -1.766 & 1.217 & 0.549 & 0.817 & -0.164 & -0.784 \\ -1.186 & 0.818 & 0.368 & 0.549 & -0.110 & -0.527 \end{pmatrix}, \tag{A 2}$$

Table 7. Linear piezoelectricity coefficients in 10^{-12}C/N

materials	non-zero piezoelectricity coefficients				
$PbNb_2O_6$ (C_{2v})	d_{31}	d_{32}	d_{33}	d_{15}	d_{24}
	−43	24	60	90	85
wood (D_2)	d_{14}	d_{25}	d_{36}		
	−0.09	0.15	0.035		
$LiTaO_3$ (C_{3v})	$d_{31}(d_{32})$	d_{22}	d_{33}	$d_{15}(d_{24})$	$d_{21} = d_{16} = -d_{22}$
	−3.0	9.0	9.0	13	
α-quartz (D_3)	d_{11}	$d_{14}(-d_{25})$	$d_{12} = d_{26} = -d_{11}$		
	2.3	−0.335			
KH_2PO_4 (D_{2d})	$d_{14}(d_{25})$	d_{36}			
	0.65	10.5			
GaAs (T_d)	d_{14}		$d_{25} = d_{36} = d_{14}$		
	1.3				
$LiIO_2$(C_6)	$d_{31}(d_{32})$	d_{33}	$d_{14}(-d_{25})$	$d_{15}(d_{24})$	
	7.3	92.7	3.65	24.65	
ZnO (C_{4v})	$d_{31}(d_{32})$	d_{33}	$d_{15}(d_{24})$		
	−5.0	12.4	−4.15		
TeO_2 (D_4)	$d_{14}(-d_{25})$				
	4.05				
fictive from KH_2PO_4 (S_4)	$d_{31}(-d_{32})$	$d_{14}(d_{25})$	$d_{15}(-d_{24})$	d_{36}	
	7.0	0.65	−0.8	10.5	
fictive from $LiTaO_3$ (D_{3h})	d_{22}		$d_{21} = d_{16} = -d_{22}$		
	9.0				

which are transformed with the elasticity tensor: $d_{ikl} = e_{imn}(\mathrm{C}^{-1})_{mnkl}$ (the IEEE Standard on Piezoelectricity, 1988). The fictive type II material with symmetry group C_s is constructed from the right-hand quartz (YXwl) with 10 independent piezoelectricity coefficients as

$$(d_{iI}) = \begin{pmatrix} 0.895 & -0.281 & -0.614 & 0 & 0 & -1.766 \\ -1.766 & 1.217 & 0.549 & 0 & 0 & -0.784 \\ 0 & 0 & 0 & 0.549 & -0.110 & 0 \end{pmatrix}. \tag{A 3}$$

The type III$^-$ material under symmetry group C_2 is taken as sucrose from Newnham [1], which has 6 independent piezoelectricity coefficients as

$$(d_{iI}) = \begin{pmatrix} 0 & 0 & 0 & 0.625 & -1.21 & 0 \\ 0 & 0 & 0 & -2.11 & 0.21 & 0 \\ 1.48 & 0.74 & -3.42 & 0 & 0 & -0.435 \end{pmatrix}. \tag{A 4}$$

In table 7 above, all the piezoelectricity coefficients are taken from Newnham [1], except for $LiIO_2$, which is from Chen *et al.* [14].

The fictive material with symmetry group C_3 is constructed from $LiTaO_3$ so that

$$(d_{iI}) = \begin{pmatrix} 6 & -6 & 0 & -16 & 13 & -9 \\ -9 & 9 & 0 & 13 & 16 & -6 \\ -3 & -3 & 9 & 0 & 0 & 0 \end{pmatrix}, \tag{A 5}$$

in which there are six independent coefficients.

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