

Full Length Research Paper

# Planes and axes of symmetry in an elastic material

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Simple proofs are obtained for the Cowin-Mehrabadi theorem for the identification of a plane of symmetry or an axis of symmetry in an elastic material. The treatment is generalized to a cartesian tensor of arbitrary rank. Necessary and sufficient conditions are found for the existence of a plane of symmetry or an axis of symmetry for a piezoelectric material. Conditions are obtained for the identification of an  $n$ -fold axis of symmetry with  $n \geq 3$ .

**Key words:** Elastic material, piezoelectric tensor, plane of symmetry, axis of symmetry, necessary and sufficient conditions.

## INTRODUCTION

Physical properties of anisotropic elastic materials are described by means of tensors, such as the dielectric tensor,  $\epsilon$ , of rank two, the piezoelectric tensor,  $\mathbf{e}$ , of rank three and the elasticity tensor,  $\mathbf{C}$ , of rank four. Components of these tensors depend on the system of coordinate axes and the tensors are usually represented in matrix form. If the crystal possesses a plane of symmetry or an axis of symmetry, and an axis of a rectangular coordinate system is chosen to be parallel to the normal to the plane of symmetry or the axis of symmetry, the matrix representing the tensor acquires a simple form in which several components vanish and relations among others become apparent. However, with reference to an arbitrary coordinate system, the components exhibit none of these features and it is not obvious whether or not the crystal belongs to any of the symmetry classes characterizing elastic materials. For a plane of symmetry, Cowin and Mehrabadi (1987) addressed this problem. Let  $C_{ijkl}$ ,  $i, j, k = 1, 2, 3$  denote components of the elasticity tensor. They proved the following theorem.

## Theorem 1

A set of necessary and sufficient conditions for a unit vector  $\mathbf{n}$  to be normal to a plane of symmetry is that it should be a common eigenvector of the following tensors:

$$U_{ij} = C_{ijkk},$$

$$V_{ij} = C_{ikjk},$$

$$W_{ik}(\mathbf{n}) = C_{ijks} n_j n_s,$$

$$W_{ik}(\mathbf{m}) = C_{ijks} m_j m_s,$$

where  $\mathbf{m}$  is any vector lying in the symmetry plane, summation on the repeated indices is understood and free indices take values 1, 2, 3.

Cowin (1989) later showed that the aforementioned conditions can be modified, so that  $\mathbf{n}$  can be a common eigenvector of the last two of the aforementioned four tensors. Ting (1996, 2003) improved the aforementioned result to hold for any one  $\mathbf{m}$ , rather than an arbitrary vector in the plane of symmetry. A vector,  $\mathbf{p}$ , is called a  $k$ -fold axis of symmetry,  $A_k$ , if a crystal is invariant with respect to rotation through an angle  $2\pi/k$ . The tensor,  $\mathbf{Q}$ , associated with rotation of a rigid body about an axis  $\mathbf{p}$  by an angle  $\theta$  is given by:

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$$\mathbf{Q} = \mathbf{I} + \sin \theta \mathbf{P} + (1 - \cos \theta) \mathbf{P}^2, \quad (1)$$

where the tensor  $\mathbf{P} = (P_{ij})$  is defined as  $P_{ij} = -\varepsilon_{ijk} p_k$ , and  $\mathbf{I}$  denotes the unit tensor  $\delta_{ij}$  (Goldstein et al., 2006; Mehrabadi et al., 1995). The corresponding tensor  $\mathbf{\Omega}$ , for reflection in a plane of symmetry with normal  $\mathbf{n}$ , is relatively simple and is given by:

$$\Omega_{ij} = \delta_{ij} - 2n_i n_j. \quad (2)$$

Ahmad (2010) used properties of  $\mathbf{Q}$  to prove.

**Theorem 2**

For a unit vector  $\mathbf{p}$  to be an axis of symmetry of an elastic material, it is necessary that it is an eigenvector of  $\mathbf{U}$ ,  $\mathbf{V}$  and  $W_{ik}(\mathbf{p}) = C_{ijks} p_j p_s$ .

Case of an  $A_3$  axis needs special treatment, but if  $\mathbf{p}$  is an  $A_2$ ,  $A_4$  or  $A_6$  axis, Theorem 1, with  $\mathbf{n}$  replaced

by  $\mathbf{p}$  provides necessary and sufficient conditions for  $\mathbf{p}$  to be an axis of symmetry. Properties of a piezoelectric material are described by means of a tensor,  $e_{ijk}$ , which has rank 3 and is symmetric with respect to the last two indices, that is,  $e_{ijk} = e_{ikj}$ . Because of this symmetry, the tensor has 18 independent components. It is convenient to represent it in the form of the following  $3 \times 6$  matrix:

$$\mathbf{e} = \begin{bmatrix} e_{11} & e_{12} & e_{13} & e_{14} & e_{15} & e_{16} \\ e_{21} & e_{22} & e_{23} & e_{24} & e_{25} & e_{26} \\ e_{31} & e_{32} & e_{33} & e_{34} & e_{35} & e_{36} \end{bmatrix}, \quad (3)$$

where the familiar two-index notation is used. Thus  $e_{11} = e_{111}$ ,  $e_{14} = e_{123} = e_{132}$ ,  $e_{15} = e_{113} = e_{131}$ ,  $e_{16} = e_{112} = e_{121}$ , etc.

Proofs of Theorems 1 and 2 and other results dealing with planes or axes of symmetry normally utilize properties of the tensors  $\mathbf{\Omega}$  or  $\mathbf{Q}$  to find invariant tensors of rank 2 with respect to coordinate transformations representing a reflection in a plane or a rotation about an axis. For example, each of the four tensors in Theorem 1 is invariant under the transformation, therefore each of them must have  $\mathbf{n}$  as an eigenvector (Ahmad and Khan, 2009). In this paper, first

we shall provide somewhat simple and short proofs of necessary conditions in Theorems 1 and 2 by searching for invariant directions associated with the elasticity tensor. In case of a plane of symmetry, such a direction must be orthogonal to  $\mathbf{n}$ , whereas in case of an axis of symmetry, it must be parallel to  $\mathbf{p}$ . This approach immediately generalizes to tensors of arbitrary rank and produces elegant results for the piezoelectric tensor. We shall also present a set of necessary and sufficient conditions for the existence of an axis of symmetry of an order greater than or equal to 3.

**NECESSARY AND SUFFICIENT CONDITIONS FOR A NORMAL OR AN AXIS OF SYMMETRY**

Suppose a plane of symmetry exists with  $\mathbf{n}$  as normal. With respect to the transformation associated with the plane of symmetry, every vector parallel to  $\mathbf{n}$  reverses its direction but any vector orthogonal to  $\mathbf{n}$  is transformed into itself. Conversely if a vector reverses its direction, it cannot have a component in the plane orthogonal to  $\mathbf{n}$ ; hence, it must be parallel to  $\mathbf{n}$ . Now, consider the vector  $U_{ij} n_j$ . This vector will transform as:

$$\begin{aligned} (U_{ij} n_j)' &= U'_{ij} n'_j = U_{ij} (-n_j) \\ &= -U_{ij} n_j. \end{aligned} \quad (4)$$

Hence,  $U_{ij} n_j$  is parallel to  $n_i$ , which implies  $\mathbf{n}$  is an eigenvector of the tensor  $\mathbf{U}$ . In a similar manner, it follows that  $\mathbf{n}$  is an eigenvector of  $\mathbf{V}$ . Now, it is clear that:

$$\begin{aligned} (C_{ijks} n_j n_k n_s)' &= C'_{ijks} n'_j n'_k n'_s \\ &= C_{ijks} (-n_j)(-n_k)(-n_s) \\ &= -C_{ijks} n_j n_k n_s. \end{aligned}$$

Thus, the vector  $C_{ijks} n_j n_k n_s$  reverses its direction and it must be parallel to  $n_i$  which implies that  $\mathbf{n}$  is an eigenvector of each of the tensors  $C_{ijks} n_j n_s, C_{ijks} n_k n_s$ . Finally, since  $(C_{ijks} m_j n_j m_s)' = -C_{ijks} m_j n_j m_s$ , it follows that the vector  $C_{ijks} m_j n_j m_s$  is parallel to  $n_i$ , and hence  $\mathbf{n}$  is an eigenvector of  $C_{ijks} m_j m_s$ .

With respect to the transformation associated with an axis of symmetry,  $\mathbf{p}$ , a vector transforms into itself if and only if it is parallel to  $\mathbf{p}$ . Consider the vector  $U_{ij} p_j$ .

Since  $(U_{ij}p_j)' = U_{ij}p_j$ , it follows that the vector  $U_{ij}p_j$  is parallel to  $p_i$  leading to the result that  $\mathbf{p}$  is an eigenvector of  $\mathbf{U}$ . A similar conclusion holds for the tensor  $\mathbf{V}$ . Also, since  $(C_{ijkl}p_jp_kp_l)' = C_{ijkl}p_jp_kp_l$ , the vector  $C_{ijkl}p_jp_kp_l$  is parallel to  $p_i$ , hence  $\mathbf{p}$  must be an eigenvector of  $C_{ijkl}p_jp_k$  as well as  $C_{ijkl}p_jp_l$ .

**Conditions for an  $A_n$ ,  $n \geq 3$**

If a tensor  $\mathbf{A}$  of rank two is invariant with respect to rotation through an angle  $2\pi/n$ ,  $n = 3, 4, 6$  about  $x_3$ -axis, then its matrix representation is of the form (Royer and Dieulesaint, 2000):

$$(\mathbf{A}) = \begin{bmatrix} a_{11} & a_{12} & 0 \\ -a_{12} & a_{11} & 0 \\ 0 & 0 & a_{33} \end{bmatrix}. \tag{5}$$

Thus, any tensor of rank 2 associated with the elasticity tensor will have the aforementioned representation. The following theorem uses this fact to characterize an axis of symmetry of order higher than 2. The theorem enumerates a set of necessary conditions for a vector  $\mathbf{p}$  to be an axis of symmetry  $A_n$ ,  $n = 3, 4$  or 6. We recall a result of Ahmad (2010) that if  $\mathbf{p}$  is an axis of symmetry  $A_n$ ,  $n \geq 3$ , it must be an eigenvector of both  $\mathbf{U}$  and  $\mathbf{V}$  belonging, in each case, to a nondegenerate eigenvalue.

**Theorem 3**

A set of necessary conditions for a unit vector  $\mathbf{p}$  to be an  $n$ -fold axis of symmetry,  $A_n$ ,  $n \geq 3$ , is the following.

1.  $\mathbf{p}$  is a common eigenvector of  $\mathbf{U}$  and  $\mathbf{V}$ , belonging to a nondegenerate eigenvalue.
2. With coordinate axes chosen so that  $x_3$ -axis is along  $\mathbf{p}$ , matrices representing the tensors  $\mathbf{U} = C_{iikl}$ ,  $\mathbf{V} = C_{ijkj}$ ,  $\mathbf{W}_1(\mathbf{p}) = C_{ijkl}p_kp_l$  and  $\mathbf{W}_2(\mathbf{p}) = C_{ijkl}p_jp_l$  are of the form (Equation 5).

**Proof**

Proof of the first condition being necessary is contained in the observations following (Equation 4). Since each of the four second rank tensors is invariant with respect to a transformation associated with a three fold, four fold or a six fold axis, the matrix representation must be of the form (Equation 5). Note that, if we compare a symmetric matrix,  $M = (m_{ij})$ , with Equation 5, it implies the matrix must be diagonal with  $m_{11} = m_{22}$ . However, the corresponding necessary and sufficient conditions for the piezoelectric tensor require comparison with a non-symmetric matrix ( $\mathbf{W}_3$  in Theorem 7).

The aforementioned conditions are not sufficient for the existence of an  $A_n$ ,  $n \geq 3$ . We have to separately consider  $n = 3, 4$  or 6. One or more extra conditions from the following set are required in each case.

- (a)  $c_{16} = 0$ ,  $c_{66} = \frac{c_{11} - c_{12}}{2}$ ,
- (b)  $\mathbf{p}$  is an eigenvector of  $C_{ijkl}m_jm_l$ .

Now we are able to formulate necessary and sufficient conditions for each of  $n = 3, 4$  and 6.

**Theorem 4**

Necessary and sufficient conditions for a unit vector  $\mathbf{p}$  to be a 3-fold axis of symmetry are conditions 1 and 2 of Theorem 3 and condition (a).

**Theorem 5**

Necessary and sufficient conditions for a unit vector  $\mathbf{p}$  to be a 4-fold axis of symmetry are conditions 1 and 2 of Theorem 3 and condition (b).

**Theorem 6**

Necessary and sufficient conditions for a unit vector  $\mathbf{p}$  to be a 6-fold axis of symmetry are conditions 1 and 2 of Theorem 3 and conditions (a) and (b)

**Proof**

We choose  $x_3$ -axis along  $\mathbf{p}$  and consider the matrix

representation of the tensor  $C_{ijkl}p_k p_l = C_{ij33}$ . Its matrix representation, in the two index notation, is:

$$\begin{bmatrix} c_{13} & c_{36} & c_{35} \\ c_{36} & c_{23} & c_{34} \\ c_{35} & c_{34} & c_{33} \end{bmatrix}.$$

A comparison with Equation 5 gives:

$$c_{34} = c_{35} = c_{36} = 0, \quad c_{13} = c_{23}. \tag{6}$$

Matrix representation of the tensor  $C_{ijkl}p_j p_l = C_{i3k3}$  is:

$$\begin{bmatrix} c_{55} & c_{45} & c_{35} \\ c_{45} & c_{44} & c_{34} \\ c_{35} & c_{34} & c_{33} \end{bmatrix},$$

which leads to:

$$c_{45} = 0, \quad c_{44} = c_{55}. \tag{7}$$

The tensor  $C_{ikjk}$  has the representation:

$$\begin{bmatrix} c_{11} + c_{66} + c_{55} & c_{16} + c_{26} + c_{45} & c_{15} + c_{46} + c_{35} \\ c_{16} + c_{26} + c_{45} & c_{66} + c_{22} + c_{44} & c_{56} + c_{24} + c_{34} \\ c_{15} + c_{46} + c_{35} & c_{56} + c_{24} + c_{34} & c_{55} + c_{44} + c_{33} \end{bmatrix}.$$

Comparison with Equation 5 and use of Equations 6 and 7 leads to  $c_{16} + c_{26} = 0$ ,  $c_{15} + c_{46} = 0$ ,  $c_{24} + c_{56} = 0$  and  $c_{11} = c_{22}$ . A similar comparison with  $C_{ikkl}$  leads to further relations  $c_{15} + c_{25} = 0$  and  $c_{14} + c_{24} = 0$ .

The  $6 \times 6$  matrix representation of the elasticity tensor becomes:

$$\begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ c_{12} & c_{11} & c_{13} & -c_{14} & -c_{15} & -c_{16} \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ c_{14} & -c_{14} & 0 & c_{44} & 0 & -c_{15} \\ c_{15} & -c_{15} & 0 & 0 & c_{44} & c_{14} \\ c_{16} & -c_{16} & 0 & -c_{15} & c_{14} & c_{66} \end{bmatrix}. \tag{8}$$

If condition (a) also holds, the foregoing matrix will become:

$$\begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & 0 \\ c_{12} & c_{11} & c_{13} & -c_{14} & -c_{15} & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ c_{14} & -c_{14} & 0 & c_{44} & 0 & -c_{15} \\ c_{15} & -c_{15} & 0 & 0 & c_{44} & c_{14} \\ 0 & 0 & 0 & -c_{15} & c_{14} & \frac{c_{11}-c_{12}}{2} \end{bmatrix},$$

which shows the material possesses trigonal symmetry. This proves Theorem 4.

To prove Theorem 5, we choose  $x_1$  axis along  $\mathbf{m}$ .

Tensor  $C_{ijkl}m_j m_l$  becomes  $C_{i1k1}$ , which has the matrix representation:

$$\begin{bmatrix} c_{11} & c_{16} & c_{15} \\ c_{61} & c_{66} & c_{65} \\ c_{51} & c_{56} & c_{55} \end{bmatrix}.$$

Since  $\mathbf{p} = (0, 0, 1)^T$  is an eigenvector of the foregoing matrix, we must have  $c_{15} = c_{65} = 0$ . But  $c_{65} = c_{56} = c_{14}$ . With  $c_{14} = c_{15} = 0$ , matrix of Equation 8 becomes:

$$\begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & c_{16} \\ c_{12} & c_{11} & c_{13} & 0 & 0 & -c_{16} \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ c_{16} & -c_{16} & 0 & 0 & 0 & c_{66} \end{bmatrix},$$

which is the matrix representation of the elasticity tensor with an  $A_4$  axis of symmetry (Royer and Dieulesaint, 2000). This proves Theorem 5. Theorem 6 follows on the same lines, since if both (a) and (b) hold, matrix of equation 8 will become:

$$\begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{c_{11}-c_{12}}{2} \end{bmatrix}$$

which characterizes the hexagonal symmetry.

Let  $\mathbf{q} = (\cos \alpha \sin \beta, \sin \alpha \sin \beta, \cos \beta)^T$ . The transformation:

$$\mathbf{R} = \begin{bmatrix} \cos \beta & 0 & -\sin \beta \\ 0 & 1 & 0 \\ \sin \beta & 0 & \cos \beta \end{bmatrix} \begin{bmatrix} \cos \alpha & \sin \alpha & 0 \\ -\sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} \cos \alpha \cos \beta & \sin \alpha \cos \beta & -\sin \beta \\ -\sin \alpha & \cos \alpha & 0 \\ \cos \alpha \sin \beta & \sin \alpha \sin \beta & \cos \beta \end{bmatrix}, \tag{9}$$

is such that  $\mathbf{Rq} = (0, 0, 1)^T$ . Thus,  $\mathbf{R}$  orients an arbitrary vector specified by its Euler angles  $\alpha$  and  $\beta$  along  $x_3$ -axis.

**PLANE OF SYMMETRY OF A PIEZOELECTRIC MATERIAL**

The argument leading to and following Equation 4 will now be applied to the piezoelectric tensor  $\mathbf{e}$  to find necessary and sufficient conditions for the existence of a plane of symmetry.

**Theorem 7**

Let  $\mathbf{n}$  and  $\mathbf{m}$  be unit vectors orthogonal to each other. It is necessary and sufficient for  $\mathbf{n}$  to be a normal to a plane of symmetry of a piezoelectric material that:

- (a) It is orthogonal to each of the vectors  $\mathbf{v}_1 = e_{kij}$ ,  $\mathbf{v}_2 = e_{ijk}$ ,  $\mathbf{v}_3(\mathbf{n}) = e_{ijk}n_in_j$ ,
- (b) It is parallel to each of the vectors  $\mathbf{w}_1(\mathbf{n}, \mathbf{m}) = e_{ijk}n_im_j$ ,  $\mathbf{w}_2(\mathbf{n}, \mathbf{m}) = e_{ijk}m_in_j$ ,  $\mathbf{w}_3 = e_{kij}m_in_j$ .

**Proof**

First suppose a plane of symmetry exists with normal  $\mathbf{n}$ . Under the transformation associated with this plane, consider  $\mathbf{v}_1 = \delta_{ij}e_{kij}$ :

$$\mathbf{v}'_1 = (\delta_{ij}e_{kij})' = \delta_{ij}e_{kij} = \mathbf{v}_1.$$

Thus,  $\mathbf{v}_1$  transforms into itself, hence it must be orthogonal to  $\mathbf{n}$ . Proofs of orthogonality of  $\mathbf{n}$  to  $\mathbf{v}_2$  and  $\mathbf{v}_3$  are similar.

Next, consider the transformation of  $\mathbf{w}_1(\mathbf{n}, \mathbf{m})$ . We have:

$$(e_{ijk}n_im_j)' = e_{ijk}(-n_i)m_j,$$

Thus,  $\mathbf{w}_1(\mathbf{n}, \mathbf{m})' = -\mathbf{w}_1(\mathbf{n}, \mathbf{m})$  leading to the conclusion that it must be parallel to  $\mathbf{n}$ . Similarly, it can be shown that  $\mathbf{n}$  is also parallel to  $\mathbf{w}_2(\mathbf{n}, \mathbf{m})$  and  $\mathbf{w}_3(\mathbf{n}, \mathbf{m})$ .

To show that the conditions of Theorem 7 are sufficient, choose coordinate axes so that  $x_1$  and  $x_3$  axes are, respectively aligned with  $\mathbf{m}$  and  $\mathbf{n}$ , that is,  $\mathbf{m} = (1, 0, 0)^T$  and  $\mathbf{n} = (0, 0, 1)^T$ . The condition that  $\mathbf{n}$  be orthogonal to each of  $\mathbf{v}_1, \mathbf{v}_2$  and  $\mathbf{v}_3$  leads to the following :

$$\begin{aligned} e_{31} + e_{32} + e_{33} &= 0, \\ e_{15} + e_{24} + e_{33} &= 0, \\ e_{33} &= 0. \end{aligned} \tag{10}$$

Vectors  $\mathbf{w}_1(\mathbf{n}, \mathbf{m})$ ,  $\mathbf{w}_2(\mathbf{n}, \mathbf{m})$  and  $\mathbf{w}_3(\mathbf{n}, \mathbf{m})$ , respectively become  $(e_{31}, e_{36}, e_{35})^T$ ,  $(e_{15}, e_{14}, e_{13})^T$  and  $(e_{15}, e_{25}, e_{35})^T$ . Since  $\mathbf{n}$  is parallel to each of them, we conclude that:

$$\begin{aligned} e_{31} = e_{36} &= 0, \\ e_{15} = e_{14} &= 0, \\ e_{15} = e_{25} &= 0. \end{aligned} \tag{11}$$

Equations 10 and 11 together imply:

$$e_{14} = e_{15} = e_{24} = e_{25} = e_{31} = e_{32} = e_{33} = e_{36} = 0,$$

which reduces the matrix (Equation 3) to a form so that the tensor  $\mathbf{e}$  has  $x_3$ -axis as a normal to a plane of symmetry (Royer and Dieulesaint, 2000).

**Example 1**

Consider the following  $3 \times 6$  matrix representing a piezoelectric tensor  $\mathbf{d}$ ,

$$\mathbf{d} = \begin{bmatrix} 4.7754 & -1.6177 & -2.6007 & -1.9427 & -0.13572 & -4.2248 \\ -1.7186 & 0.34562 & -0.49744 & 5.3860 & 3.4468 & 0.75776 \\ -0.10442 & -0.77998 & 1.1023 & -7.7468 & -3.0673 & -0.60562 \end{bmatrix}, \tag{12}$$

where components are in units of  $C/m^2$ . Note that

$d_{i\alpha} = d_{ijk}$ , if  $\alpha \leq 3$  and  $d_{i\alpha} = 2d_{ijk}$ , if  $\alpha > 3$  (Royer and Dieulesaint, 2000).

We wish to determine whether or not a plane of symmetry exists. Vectors  $\mathbf{v}_1$  and  $\mathbf{v}_2$  can be readily obtained from Equation 12 as:

$$\mathbf{v}_1 = (0.557023, -1.87039, 0.217873)^T \text{ and}$$

$$\mathbf{v}_2 = (3.62065, -5.64022, 3.72743)^T.$$

If there is a plane of symmetry, then its normal  $\mathbf{n}$  must be given by:

$$\mathbf{n} = \frac{\mathbf{v}_1 \times \mathbf{v}_2}{|\mathbf{v}_1 \times \mathbf{v}_2|}$$

$$= (-.830497, -0.186178, 0.524988)^T,$$

and we can take  $\mathbf{m}$  a unit vector along  $\mathbf{v}_1$ ,

$$\mathbf{m} = \frac{\mathbf{v}_1}{|\mathbf{v}_1|}$$

$$= (0.28366, -0.952485, 0.11095)^T.$$

We can now compute the vector  $\mathbf{v}_3$  which comes out as  $\mathbf{v}_3 = (2.22809, -2.33557, 2.69643)^T$ , which is orthogonal to  $\mathbf{n}$ , because  $\mathbf{n} \cdot \mathbf{v}_3 = 0$ .

Similarly, we can compute unit vectors along  $\mathbf{w}_1$ ,  $\mathbf{w}_2$  and  $\mathbf{w}_3$ , each of which is found to be  $(-0.830497, -0.186178, 0.524988)^T$ , a vector identical to  $\mathbf{n}$ . We conclude that a plane of symmetry exists, with normal  $\mathbf{n} = (-0.830497, -0.186178, 0.524988)^T$ .

If we choose  $\alpha = 3.36212$  and  $\beta = 1.0181$ , then  $\mathbf{n} = (\cos \alpha \sin \beta, \sin \alpha \sin \beta, \cos \beta)^T$ . Application of the transformation of Equation 9 to  $\mathbf{n}$ , transforms it to  $(0, 0, 1)^T$ . Same transformation applied to the tensor represented by Equation 12 leads to the standard form of the tensor for a monoclinic material with the normal to the plane of symmetry parallel to  $x_3$ -axis, that is:

$$\mathbf{d}' = \begin{bmatrix} 1.60894 & 0.72657 & -2.59149 & 0 & 0 & 3.70196 \\ -1.48785 & -0.17272 & 3.60752 & 0 & 0 & -2.82030 \\ 0 & 0 & 0 & 2.76639 & -3.16813 & 0 \end{bmatrix}.$$

With coordinate axes so that  $x_2$ -axis is along  $\mathbf{n}$ , the tensor of Equation 12 transforms to:

$$\mathbf{d}'' = \begin{bmatrix} 1.4 & 3.8 & -4.2 & 0 & -7.2 & 0 \\ 0 & 0 & 0 & -2.6 & 0 & 8 \\ -0.22 & -2.3 & 0.83 & 0 & 2.2 & 0 \end{bmatrix}$$

which is the tensor representing the yttrium calcium oxyborate (YCOB) crystal reported (Shimuzu et al., 2009).

### AXIS OF SYMMETRY OF A PIEZOELECTRIC MATERIAL

The following theorem provides necessary and sufficient conditions for a vector  $\mathbf{p}$  to be at least a 2-fold axis of symmetry. However, since a four fold or a six fold axis is also a dyad axis, conditions of the theorem will be satisfied in case of an  $A_4$  or an  $A_6$  axis as well.

Necessary and sufficient conditions for an axis  $A_n$ ,  $n \geq 3$  will be given in Theorems 9 and 10.

#### Theorem 8

Let  $\mathbf{p}$  and  $\mathbf{m}$  be unit vectors orthogonal to each other. It is necessary and sufficient for  $\mathbf{p}$  to be a 2-fold axis of symmetry of a piezoelectric material that it is parallel to each of the vectors,  $\mathbf{v}_1 = e_{ij}$ ,  $\mathbf{v}_2 = e_{ijk}$ ,  $\mathbf{v}_3(\mathbf{p}) = e_{ijk} p_i p_j$ ,  $\mathbf{v}_4(\mathbf{p}) = e_{ijk} p_j p_k$ ,  $\mathbf{v}_5(\mathbf{m}) = e_{ijk} m_i m_j$  and  $\mathbf{v}_6(\mathbf{m}) = e_{ijk} m_j m_k$

#### Proof

Proof of the Theorem 8 is similar to that of Theorem 4. Here, the transformation associated with rotation about an axis  $\mathbf{p}$  is represented by the operator  $\mathbf{Q} = -\mathbf{I} + 2\mathbf{p} \otimes \mathbf{p}$ , where  $\mathbf{I}$  is the identity operator (Ahmad, 2010).

#### Example 2

Consider the following  $3 \times 6$  matrix representation of the piezoelectric tensor  $\mathbf{e}$  corresponding to a hypothetical material.

$$\mathbf{e} = \begin{bmatrix} -0.756897 & 1.55523 & -1.59723 & 0.0815332 & -0.299296 & 0.138140 \\ 1.52488 & -0.699927 & -1.65214 & 0.296613 & -0.0961851 & 0.222583 \\ -1.79313 & 1.78259 & 0.007407 & 1.80617 & 1.73614 & -0.068369 \end{bmatrix}, \tag{13}$$

where the components are in units of  $C/m^2$ . Note that, unlike the tensor  $\mathbf{d}$  used in Example 2, for  $\mathbf{e}$ ,  $e_{i\alpha} = e_{ijk}$ ,  $i = 1, \dots, 3$ ,  $\alpha = 1, \dots, 6$ .

We wish to determine whether or not an axis of symmetry exists. Vectors  $\mathbf{v}_1$  and  $\mathbf{v}_2$  can be obtained from Equation 13 as:

$$\mathbf{v}_1 = (-0.798903, -0.827191, -0.0031403)^T,$$

$$\mathbf{v}_2 = (1.20183, 1.24438, 0.0047241)^T.$$

If  $\mathbf{p}$  is a unit vector along  $\mathbf{v}_2$  then,

$$\begin{aligned} \mathbf{p} &= \frac{\mathbf{v}_2}{|\mathbf{v}_2|} \\ &= (0.694698, 0.719296, 0.002731)^T. \end{aligned}$$

We take  $\mathbf{m}$  a unit vector orthogonal to  $\mathbf{p}$ :

$$\mathbf{m} = (0.719299, -0.694701, 0)^T.$$

Vectors  $\mathbf{v}_3$ ,  $\mathbf{v}_4$ ,  $\mathbf{v}_5$  and  $\mathbf{v}_6$  are computed as:

$$\mathbf{v}_3 = (0.576599, 0.597016, 0.0022665)^T,$$

$$\mathbf{v}_4 = \mathbf{v}_3,$$

$$\mathbf{v}_5 = (-1.1152, -1.15469, -0.0043836)^T,$$

$$\mathbf{v}_6 = (0.220898, 0.22872, 0.0008683)^T.$$

It is easily verified that:

$$\frac{-\mathbf{v}_1}{|\mathbf{v}_1|} = \frac{\mathbf{v}_2}{|\mathbf{v}_2|} = \frac{\mathbf{v}_3}{|\mathbf{v}_3|} = \frac{-\mathbf{v}_5}{|\mathbf{v}_5|} = \frac{\mathbf{v}_6}{|\mathbf{v}_6|} = \mathbf{p}.$$

This shows that  $\mathbf{p} = (0.694698, 0.719296, 0.002731)^T$  is indeed an axis of symmetry. Angles  $\alpha$  and  $\beta$  pertaining to  $\mathbf{p}$  are respectively 0.802793 and 1.56807 and the transformation matrix of Equation 9 becomes:

$$\begin{bmatrix} 0.0018970 & 0.0019642 & -0.999996 \\ -0.719299 & 0.694701 & 0 \\ 0.694698 & 0.719296 & 0.002731 \end{bmatrix}. \quad (14)$$

The aforementioned transformation aligns  $\mathbf{p}$  along  $x_3$ -axis and, with respect to the new coordinate axes, the

piezoelectric tensor has the following matrix representation:

$$\begin{bmatrix} 0 & 0 & 0 & -1.78917 & 2.5053 & 0 \\ 0 & 0 & 0 & -1.6053 & -0.20917 & 0 \\ -2.29798 & 0.317977 & 0.83 & 0 & 0 & -0.386904 \end{bmatrix},$$

which shows that the material has an  $A_2$  axis parallel to  $x_3$ -axis.

The following theorem concerning the piezoelectric tensor is the counterpart of Theorems 4 to 6 for the elasticity tensor.

### Theorem 9

A set of necessary and sufficient conditions for a unit vector  $\mathbf{p}$  to be a three fold axis of symmetry for a piezoelectric material described by the tensor  $\mathbf{e} = (e_{ijk})$ , is the following.

1.  $\mathbf{p}$  is parallel to  $\mathbf{v}_1 = e_{ijj}$  as well as  $\mathbf{v}_2 = e_{jji}$ .
2. With coordinate axes chosen so that  $x_3$ -axis is along  $\mathbf{p}$ , the matrices representing second rank tensors  $\mathbf{W}_3 = e_{ijk} p_k$  and  $\mathbf{W}_4 = e_{ijk} p_i$  are of the form (Equation 5).

### Proof

Proof of the necessity of the conditions is easy. We will show that the conditions are sufficient. Choose  $x_3$ -axis parallel to  $\mathbf{p}$ ,  $\mathbf{p} = (0, 0, 1)^T$ . Since  $\mathbf{v}_1$  is parallel to  $\mathbf{p}$ , we conclude that:

$$\begin{aligned} e_{11} + e_{12} + e_{13} &= 0, \\ e_{21} + e_{22} + e_{23} &= 0. \end{aligned} \quad (15)$$

Similarly  $\mathbf{v}_2$  is parallel to  $\mathbf{p}$ , leads to:

$$\begin{aligned} e_{11} + e_{26} + e_{35} &= 0, \\ e_{16} + e_{22} + e_{34} &= 0. \end{aligned} \quad (16)$$

Matrices representing the tensors  $\mathbf{W}_3$  and  $\mathbf{W}_4$  are as follows:

$$\mathbf{W}_3 = \begin{bmatrix} e_{15} & e_{14} & e_{13} \\ e_{25} & e_{24} & e_{23} \\ e_{35} & e_{34} & e_{33} \end{bmatrix},$$

$$\mathbf{W}_4 = \begin{bmatrix} e_{31} & e_{36} & e_{35} \\ e_{36} & e_{32} & e_{34} \\ e_{35} & e_{34} & e_{33} \end{bmatrix}.$$

Comparison with Equation 5, leads to:

$$\begin{aligned} e_{15} &= e_{24}, e_{14} = -e_{25}, \\ e_{13} &= e_{23} = e_{34} = e_{35} = 0, \\ e_{31} &= e_{32}, e_{36} = -e_{36} = 0. \end{aligned} \tag{17}$$

Equations 15 to 17 imply that there are only six independent components of the tensor  $\mathbf{e}$  and it will have the representation:

$$\begin{bmatrix} e_{11} & -e_{11} & 0 & e_{14} & e_{15} & -e_{22} \\ -e_{22} & e_{22} & 0 & e_{15} & -e_{14} & -e_{11} \\ e_{31} & e_{31} & e_{33} & 0 & 0 & 0 \end{bmatrix}, \tag{18}$$

which is the form of a tensor belonging to a trigonal material (Royer and Dieulesaint, 2000). Thus, the material has trigonal symmetry. Finally we have the following theorem

**Theorem 10**

Let  $\mathbf{m}$  and  $\mathbf{n}$  be mutually perpendicular unit vectors in the plane normal to  $\mathbf{p}$ . If, in addition to conditions (1) and (2) of Theorem 9, the tensor  $e_{ijk}$  satisfies the condition:

$$3. e_{ijk} m_i n_j + e_{ijk} m_j n_i = 0,$$

Then  $\mathbf{p}$  is a four fold or a six fold axis of symmetry.

**Proof**

We can choose  $x_1$  and  $x_2$  axes, respectively along  $\mathbf{m}$  and  $\mathbf{n}$ . Condition (3) of the Theorem becomes  $e_{12k} + e_{21k} = 0$ . Thus  $e_{16} = -e_{21}, e_{12} = -e_{26}, e_{14} = -e_{25}$ . Use of these conditions in equation 18, leads to  $e_{11} = e_{22} = 0$  and matrix becomes:

$$\begin{bmatrix} 0 & 0 & 0 & e_{14} & e_{15} & 0 \\ 0 & 0 & 0 & e_{15} & -e_{14} & 0 \\ e_{31} & e_{31} & e_{33} & 0 & 0 & 0 \end{bmatrix},$$

which is precisely the matrix representation of the piezoelectric tensor possessing tetragonal or hexagonal symmetry.

**Conclusions**

The results developed in this paper are capable of immediate generalization to a tensor of arbitrary rank. In some applications, tensors of rank higher than 4 are required to adequately model the physical phenomena. For example Ozarslam and Mareci (2003) have noted that the diffusion tensor of rank 2 has limited application in the modeling of diffusion imaging and have proposed the use of the diffusion tensors of rank going up to 8. Taking a cue from this observation, let us consider a tensor  $\mathbf{T}$  of rank 6 which describes some physical property of a material possessing a plane of symmetry with normal  $\mathbf{n}$ . Then, the following necessary conditions must hold.

1.  $\mathbf{n}$  is an eigenvector of each of the tensors of rank 2 obtained from  $\mathbf{T}$  by letting any pair of indices free and contracting others in pairs. For example  $T_{ijkll}, T_{klijl}$ , are two of such tensors.
2.  $\mathbf{n}$  is an eigenvector of the tensor obtained by contracting any three pairs of indices of  $T_{ijklmn} n_p n_q$  or any four pairs of  $T_{ijklmn} n_p n_q n_r n_s$ .

Similar results concerning an axis of symmetry will also hold.

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